93RD ANNUAL MEETING

of the International Association of Applied Mathematics and Mechanics

TECHNISCHE UNIVERSITÄT DRESDEN

May 30th – June 2nd, 2023
Dresden (Germany)

100 JAHRE GAMM

Book of Abstracts

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Book of Abstracts of the
93rd Annual Meeting
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Contents

Prandtl Memorial Lecture, Plenary and Public Lectures

Ludwig Prandtl Memorial Lecture

Date: May 30, 2023 10:00-11:00
Room: Hörsaalzentrum (AUDIMAX)
Laudation: Martin Oberlack

Data-driven modeling of fluid flows

Clarence W. Rowley *(Princeton University, USA)*

Fluid flows can be extraordinarily complex, and even turbulent, yet often there is structure lying within the apparent complexity. Understanding this structure can help explain observed physical phenomena, and can help with the design of control strategies in situations where one would like to change the natural state of a flow. This talk addresses techniques for obtaining simple, approximate models for complex systems such as fluids, using data from simulations or experiments. We discuss a number of methods, including principal component analysis, balanced truncation, and Koopman operator methods, and focus on a new method for optimizing projections of nonlinear systems. We apply these techniques to a number of examples, including toy models that illustrate the key modeling difficulties, as well as several flows with complex behavior, including a transitional channel flow and an axisymmetric jet.

Plenary Lecture 1

Date: May 30, 2023 11:00-11:45
Room: Hörsaalzentrum (AUDIMAX)
Chair: Stefanie Reese

A material point method for advection-diffusion problems in open systems

Anna Pandolfi *(Politecnico di Milano, Italy)*

Numerical solutions of advection-diffusion problems encounter difficulties when traditional methods based on finite element and finite difference discretization are employed. A more natural alternative is to employ material particle approximation paradigms, such as the Optimal Transportation Meshfree (OTM) method (Fedeli et al, 2017), which are geometrically exact as regards advection. The work was confined to advection-diffusion problems in closed systems, where the mass of the diffusive species is kept within a fixed container during its evolution. In particular, density sources within the domain and fluxes or assigned densities at the boundaries (homogeneous Dirichlet and Neumann boundary) were excluded from consideration and the advection field was assumed tangent to the boundary.

In this talk, we show that the OTM approach can be applied to open systems characterized by density sources or sinks and general transport boundary conditions, including prescribed fluxes and density values. We provide a semi-discrete derivation of the spatial discretization (material points and max-ent shape functions) that reduces the governing equations to a system of ordinary differential equations in time. The choice of time integration scheme is left free and can be implicit, such as the variational Wasserstain method of minimizing movements, or explicit, such as the Runge-Kutta method, or other such convenient scheme. We

also present selected test cases that illustrate these trade-offs, as well as the overall scope and convergence properties of the approach.

The study has been conducted in collaboration with Michael Ortiz and Laurent Stainer.

Plenary Lecture 2

Date: May 30, 2023 11:45-12:30
Room: Hörsaalzentrum (AUDIMAX)
Chair: Barbara Zwicknagl

Rigidity and Flexibility in the Modelling of Shape-Memory Alloys

Angkana Rüland *(University of Bonn, Germany)*

In this talk, I discuss a striking dichotomy which arises in the modelling of shape-memory alloys. This dichotomy can already be observed in the exactly stress-free setting: On the one hand, at sufficiently high regularity, solutions to the associated differential inclusions are rigid. They obey the "characteristic equations" determined by the differential inclusion and thus satisfy the associated kinematic compatibility conditions. In particular, structures such as, for instance, simple laminates or crossing twins are obtained which are also experimentally observed. On the other hand, on relaxing or on even completely dropping these regularity assumptions, the problem becomes flexible: A plethora of highly irregular, highly non-unique, "wild" solutions emerges.

In this talk, I will explore this phase transformation in the modelling of shape-memory alloys. In particular, I will discuss qualitative and quantitative analytical results on this dichotomy and will complement these with some numerical simulations. The talk is based on joint work with F. Della Porta, J. Taylor, A. Tribuzio, Ch. Zillinger and B. Zwicknagl.

Plenary Lecture 3

Date: May 31, 2023 16:30-17:15
Room: Video – Hörsaalzentrum (AUDIMAX)
Chair: Peter Benner

Alloys of AI and Computational Science

Petros Koumoutsakos *(Harvard-School of Engineering, MA, USA)*

Over the last thirty years, we have experienced more than a billion-fold increase in hardware capabilities and a dizzying pace of acquiring and transmitting massive amounts of data. Scientific Computing and Artificial Intelligence (AI) have been key beneficiaries of these advances. This talk will offer a perspective on forming algorithmic alloys of AI and simulations to predict and control complex systems.

The applications have an emphasis on fluid mechanics. Alloys will include algorithms for learning the Effective Dynamics (LED) of complex systems and a fusion of multi-agent reinforcement learning and scientific computing (SciMARL) for modeling and controlling turbulent flows. The talk will present successes and failures and argue that the proper fusion of domain knowledge and AI expertise is essential for advancing scientific frontiers.

Plenary Lecture 4

Date: May 31, 2023 17:15-18:00
Room: Video – Hörsaalzentrum (AUDIMAX)
Chair: Dennis Kochmann

Mechanics of Peeling Induced Shape Morphing in Plastic Films

Huajian Gao *(Nanyang Technological University Singapore, Singapore)*

Three-dimensional (3D) architectures have qualitatively expanded the functions of materials and electronic devices. However, current fabrication techniques for devices constrain their substrates to 2D geometries or are limited to heterogeneous or responsive materials, excluding inert plastic films such as polyethylene terephthalate (PET) and polyimide (PI) which are vital substrates for electronics. Here, we introduce peeling induced shape morphing as a versatile strategy to transform inert plastic films into various freestanding 3D structures through programming of peeling-induced plastic strain [1]. Mechanics modeling, validated by finite element simulations and experimental results, reveals the underlying mechanisms of peeling-induced shape morphing and serves as a powerful tool for the prediction and design of 3D devices obtained by the proposed approach. Some examples are used to demonstrate the potential applications of the proposed approach in making freestanding 3D devices.

Reference:

[1] F.L. Zhang, D. Li, C.X. Wang, Z.H. Liu, M. Yang, Z.Q. Cui, J.Q. Yi, M. Wang, Y. Jiang, Z.S. Lv, S.T. Wang, H.J. Gao and X.D. Chen, 2022, Nature Communications, Vol. 13, Art. No. 7294. DOI: 10.1038/s41467-022-34844-y

Plenary Lecture 5

Date: June 1, 2023 11:00-11:45
Room: Hörsaalzentrum (AUDIMAX)
Chair: Jochen Fröhlich

Fluid Mechanics under Microgravity Conditions

Christoph Egbers *(BTU Cottbus, Germany)*

The GeoFlow (Geophysical Flow) experiment on the ISS was designed to study convective processes under microgravity conditions in the spherical geometry, [1]. By applying a high voltage potential between two concentric spherical shells and utilizing a dielectric working fluid, it is possible to obtain an artificial radial force field, which is comparable to a planetary gravitational field. This makes it possible to study convection, as it occurs in the Earth's outer core or in the Earth's mantle. The visualization is realized by a Wollaston shearing interferometry unit, which is part of the Fluid Science Laboratory (FSL) of the Columbus module, [2].

Two GeoFlow missions have been performed. The first mission, GeoFlow I (2008-2009), used an iso-viscous working fluid (M5). The specific parameter regime of the experiment had similarities with convective flows which are assumed in the Earth's core. Not only the stable laminar regime, but the transition to turbulence is investigated in detail. The second mission, GeoFlow II (2011-2018), consists of three campaigns, namely GeoFlow IIa-c, using 1-Nonanol as working fluid. This alcohol has a temperature depended viscosity. [3,4].

The main objective of the new AtmoFlow experiment is the investigation of global cells and planetary waves as they are known from planetary atmospheres, [5]. Understanding the interaction between atmospheric circulation and a planet's climate, i. e. Earth, Mars, Jupiter, or a distant exoplanet, contributes to various fields of research such as astrophysics, geophysics, fluid physics, and climatology. Without losing its overall view on the complex physics, circulation in planetary atmospheres can be reduced to a simple model of a central gravitational field with a temperature gradient applied from cold polar to hot equatorial region and rotational effects.

[1] B. Futterer, A. Krebs, A.-C. Plesa, F. Zaussinger, R. Hollerbach, D. Breuer, and C. Egbers. **JFM**. 735: 647–683, Nov 2013.
[2] F. Zaussinger, A. Krebs, V. Travnikov, and C. Egbers. **Adv. Space Res.**, 60(6):1327–1344, 2017.
[3] F. Zaussinger, P. Haun, M. Neben, T. Seelig, V. Travnikov, C. Egbers, H. Yoshikawa, and I. Mutabazi. **Phys. Rev. Fluids**, 3:093501, Sep 2018.
[4] V. Travnikov, F. Zaussinger, P. Beltrame, and C. Egbers. **Phys. Rev. E**, 96(2), Aug 2017.
[5] F. Zaussinger, P. Canfield, A. Froitzheim, V. Travnikov, P. Haun, M. Meier, A. Meyer, P. Heintzmann, T. Driebe, and C. Egbers. **Microgravity. Sci. & Tech.**, Juli 2019.

Plenary Lecture 6

Date: June 1, 2023 11:45-12:30
Room: Hörsaalzentrum (AUDIMAX)
Chair: Gerlind Plonka-Hoch

Regularization by architecture: Deep Learning for PDE-based inverse problems

Peter Maaß *(University of Bremen, Germany)*

The stunning success of data driven concepts for a large variety of applications and the exponentially growing body of literature, e. g. on applications in computer vision, is still in contrast to the growing but limited knowledge of its mathematical foundations. This is even more visible for complex applications beyond image processing.

In this paper we focus on tasks in parameter identification, which are modelled as inverse problems. Such problems are typically ill-posed and a direct transfer of learned concepts such as neural networks fail. Hence we aim at combining expert knowledge in terms of physical-mathematical models with learned concepts.

The first part of the talk starts with a basic introduction on deep learning approaches to parameter identification and inverse problems. We will present mathematically proven results, which embed certain network architectures into the regularization theory for inverse problems. In particular we focus on learned ISTA concepts and describe them as a method for learning a data dependent optimized Tikhonov functional.

On the experimental side we focus on low dose CT reconstructions. We present a standardized data set and perform a numerical comparison of different deep learning concepts. The comparison is in terms of accuracy but also in terms of the amount of test data needed for training.

The second part of the talk addresses deep learning concepts for partial differential equations. We start with a survey of the most common approaches for solving PDEs and the related theory. We then focus on how to adapt those methods to PDE-based parameter identification problems.

On the experimental side we focus on industrial applications to structural mechanics (cooperation with Ariane Group) and we present our TorchPhysics research programme (cooperation with Bosch).

This is joint work with Johannes Leuschner, Maximilian Schmidt, Sören Dittmer, Daniel Otero Baguer, Clemens Arndt, Tobias Kluth, Matthias Beckmann, Nick Heilenkötter, Uwe Iben.

Plenary Lecture 7

Date: June 2, 2023 14:00-14:45
Room: Hörsaalzentrum (AUDIMAX)
Chair: Robert Seifried

Efficient Modelling – how simple can it get?

Katrin Ellermann *(Technical University Graz, Austria)*

In scientific research, modeling is a common practice used to predict or investigate the behavior of specific systems. However, it is essential to recognize that there is no "correct" model for various systems due to multiple uncertainties that can affect the model or the validation process. Instead, models can be classified based on their suitability to the system's context.

The human brain naturally attempts to simplify complex questions and problems, often by breaking them down into simpler components or characteristic patterns. This simplification process helps us identify a system's essential elements and reduce complexity to more manageable levels. Modeling is often based on initial educated guesses, which can lead to a model that can be accepted, refined, or discarded based on how well it matches the characteristics of the real system. However, it is essential to balance simplicity and accuracy when creating models. As the complexity of models increases, more effects can be captured, but the potential for errors and inaccuracies also rises. Therefore, finding the right level of complexity for a model is critical to its success. While many modeling approaches and techniques are available, it is essential to remember that a "good" model should also be a "simple" one.

Systematic approaches can be used to refine simplistic models or reduce excessively complex ones. Systematic approaches like model order reduction, uncertainty quantification, and sensitivity analysis are becoming important steps in computational modeling. These techniques have shown impressive results in refining simplistic models and reducing overly complex ones. By finding the right level of complexity for a model, researchers can reach conclusions that may not be directly attainable from complex descriptions.

In this talk, we will discuss the historical background of computational modeling, the importance of finding the right level of complexity for a model, and the various systematic approaches that can be used to achieve this. We will also explore the challenges posed by complex and nonlinear models, possible pitfalls, and the ongoing quest for easy solutions in computational modeling.

Plenary Lecture 8

Date: June 2, 2023 14:45-15:30
Room: Video – Hörsaalzentrum (AUDIMAX)
Chair: Patrick Dondl

Mean Field limits for singular flows

Sylvia Serfaty *(Courant Institute of Mathematical Sciences, NY, USA)* 14:45

Large ensembles of points with Coulomb interactions arise in various settings of condensed matter physics, classical and quantum mechanics, statistical mechanics, random matrices and even approximation theory, and they give rise to a variety of questions pertaining to analysis, Partial Differential Equations and probability.

We will first review these motivations, then present the "mean-field" derivation of effective models and equations describing the system at the macroscopic scale. We then explain how to analyze the next order behavior, giving information on the configurations at the microscopic level and connecting with crystallization questions, and finish with the description of the effect of temperature.

Public Lecture 1

Date: June 1, 2023 20:00-21:30
Room: Hörsaalzentrum (AUDIMAX)
Chair: Karsten Urban

100 Jahre GAMM: Motivation, Historie und Errungenschaften

Wolfgang Ehlers *(University of Stuttgart, Germany)*

Der Vortrag behandelt die 100-jährige Geschichte der GAMM von ihren Anfängen in den 20iger Jahren des vorigen Jahrhunderts bis heute und beleuchtet durch Beispiele die wissenschaftlichen Errungenschaften, an denen die GAMM und ihre Mitglieder mitgewirkt haben.

Public Lecture 2

Date: June 2, 2023 20:00-21:30
Room: Hörsaalzentrum (AUDIMAX)
Chair: Stefan Löhnert

Was hat das Universum mit mir zu tun?

Harald Lesch *(LMU Munich, Germany)*

Ein Spaziergang durch die empirischen, quantitativen Wissenschaften vom Kosmos, der Materie, dem Raum und der Zeit.

Harald Lesch, Professor für Astrophysik am Lehrstuhl für Astronomie und Astrophysik der LMU München ist nicht nur in der Wissenschaft sondern auch durch viele interessante Wissenschaftsfernsehsendungen, wie etwa Abenteuer Forschung, Terra-X und Leschs Kosmos in der breiten Öffentlichkeit bekannt. Durch seine faszinierende Art, komplizierte naturwissenschaftliche und technische Zusammenhänge für jeden verständlich zu erläutern, erfreut er

sich in der Bevölkerung großer Beliebtheit. In diesem astronomischen Vortrag widmet sich Harald Lesch der Frage:

Wie hat alles angefangen, wie ist es geworden und was machen wir in diesem Universum. Die große Geschichte der Natur in gut einer Stunde.

Minisymposia

MS1: Modern teaching and didactics in mathematics and mechanics

Organizer(s): **Walther, Andrea** *(Humboldt-Universität zu Berlin)*
Bartel, Thorsten *(TU Dortmund)*

MS1-01: Modern teaching and didactics in mathematics and mechanics

Date: June 1, 2023 13:30-15:30
Room: HSZ/H02

Basic concepts of didactics and examples of competence-oriented implementations.

Bartel, Thorsten *(TU Dortmund, Germany)* 13:30

Higher education in general and especially in mathematics and engineering is facing major challenges. On the one hand, the steadily increasing heterogeneity of students has to be taken into account. On the other hand, professional requirements – both in academia and industry – have changed significantly in essential aspects within a short period of time. To cope with these challenges, the implementation of sophisticated didactical concepts is urgently needed. This paper therefore explains the basic concepts such as "constructivism", "learning objectives", "taxonomy levels" and "constructive alignment". Frequently, misunderstandings and hasty conclusions regarding the feasibility of these concepts occur. For this reason, this paper also aims to dispel these misconceptions and to present and discuss concrete examples. These examples include, among others, the targeted reduction of the previous teaching content and the reorientation of various focal points, e.g., to the integration and use of computer programs and programming languages.

How to make students study during the semester

Kochmann, Dennis M. *(ETH Zurich, Switzerland)* 13:50
Franze, Andreas *(HTW Dreden University of Applied Sciences, Germany)*

We all know this problem from teaching large undergraduate classes. Our typical format of lecturing to huge student audiences and solving example problems in exercise sessions on the board has demonstrably limited effectiveness. Moreover, it often promotes that students aim to absorb information during the semester and concentrate all their studying efforts right before the exam (with the sole objective of passing the exam). Such learning is ineffective and little sustainable. What is missing is *time on task* by the students during the semester. Therefore, a key question has been: how can we make sure that our students spend quality time during the semester on actively developing a fundamental understanding as well as analytical and/or computational problem solving skills? We will discuss a number of tools that have been deployed and are being continuously developed in some of the undergraduate mechanics

courses in Mechanical Engineering at ETH Zurich and HTW Dresden, including basic mechanics classes as well as electives in computational mechanics. Key are concepts such as Flipped Classroom, Peer instruction and just-in-time teaching. The idea of the Flipped Classroom is to provide the learning material before the lecture, so that the time in the lecture is used for practical application and discussion. To this end, short video sequences are provided and online self-tests are offered to check students' understanding. Whether or not Flipped Classroom or on-site lectures are preferred, peer instruction and just-in-time teaching can then be used during the quality-time students spend in the lecture halls. In addition, we show further specific activation elements such as challenging student polls (ideally combined with an experiment or application), weekly online learning elements as homework (using gamification for advanced participation), and computational projects (translating theoretical concepts into code). Aside from making sure that students spend time on the subject, such elements also provide timely feedback to the students on their individual learning success as well as to the instructor on the collective performance. Our experience and statistics evaluation in terms of Scholarship of Teaching and Learning show that an effective combination of didactical concepts significantly enhances student activity. Furthermore, even little incentives are sufficient to maintain student participation with a positive impact on sustainable learning and exam outcomes.

Proving as a main aspect and implementing as a secondary aspect? Results of an interview study on competencies in numerical analysis courses

Burr, Laura *(Ulm University, Germany)* 14:10

Numerical analysis has (so far) played a minor role in math didactics. Although the importance of (numerical) algorithms in almost all areas of daily life is steadily growing, there are comparatively few international and national contributions dealing with the teaching, learning and examination of numerical analysis. Moreover, as pointed out in previous work, the focus of research is so far on teaching and learning numerical analysis in engineering courses and integrating numerical analysis topics in schools. Numerical analysis courses in the context of math degree programs have been studied only sporadically so far. Therefore, the identification and description of students' competencies in these courses is still pending but seems to be of particular importance especially with respect to the design of adequate and competency-based forms of teaching, learning and examination. Building on previous work, this talk presents the results of an interview study on students' competencies in numerical analysis courses. For this purpose, a total of 17 numerical analysis teachers from different universities were interviewed one-on-one in 2021 and 2022. It can be seen that the requirements for students are very diverse. For example, in addition to implementing algorithms on the computer, they should also be able to visualize, analyze, evaluate, compare, apply and select algorithms.

Above all: motivation ++ our maths-for-engineers teaching concept

Feldmann, Ute *(Technische Universität Dresden, Germany)*
Franz, Sebastian *(Technische Universität Dresden, Germany)* 14:30

We present our maths-for-engineers teaching concept:

Above all, motivation: Sometimes mathematics teachers observe that engineering students, for example, perceive the math material as a useless evil for them and therefore learn with little motivation and sustainability. If the math material is later used by other subjects, the students do not know how to apply it and the teachers do not think much of the math education.

We solve the motivation problem by linking the mathematics with other subjects: the maths exercise program contains specific tasks from application subjects at that moment when the necessary mathematical know-how is available; examples can be found here: https://www pub.zih.tu-dresden.de/~feldm/vernetzung.html.

In our contribution we will document our experience in achieving this maths-others subjects-link and the success in motivating students.

Other parts of our teaching concept are:

1. making recordings of lectures and tutorials available so that students can decide whether to attend the face-to-face lecture or watch the video at home in 'flipped-classroom-style': 4/5 of our students choose face-to-face but use the recordings for review.

2) Instead of TWO small group exercises per week, we offer ONE central exercise and ONE small group exercise per week: We are documenting the success of this change based on student views and on changes in exam scores: the pass rate did not change, but we observed a raised midfield.

3. by means of our extra credit rules: https://tu-dresden.de/mn/math/wir/ressourcen/dateien/studium/ma1/spielregelnMa1.pdf we evoke a) group work, b) that students continuously 'stay on task' throughout the semester, as well as c) keep reviewing what they have learned so far.

4. 100%-transparency about what we taught and how we taught it, see an example here: https://tu-dresden.de/mn/math/wir/ressourcen/dateien/studium/ma2/Plan_Ma2_2022.pdf. This enables teachers of follow-up subjects to use knowledge already taught effectively in their lectures.

Teaching mechanics with individual exercise assignments and automated correction

Gfrerer, Michael Helmut *(Graz University of Technology, Austria)*
Marussig, Benjamin *(Graz University of Technology, Austria)*
Maitz, Katharina *(Graz University of Technology, Austria)*
Bangerl, Mia Magdalena *(Graz University of Technology, Austria)*

14:50

The presented project aims to improve the education of engineers in mechanics. We believe that the independent solving of exercises is an indispensable part of developing a student's mechanical understanding. Yet, most mechanics lectures have more than 200 participants, and from the teacher's point of view, the effort of manually creating and correcting assignments limits the number of exercises. However, a small number of assignment examples makes it considerably more difficult to check whether students could solve them themselves. For students, on the other hand, unreflected copying of tasks already solved does not foster the understanding of the material to be learned and leads to a false self-assessment.

We address this “classical issue” of homework assignments by providing a scalable approach for creating, distributing, and correcting them.First, problem sets with a similar level of complexity are assembled by abstract modification rules and symbolically solved to obtain the reference solutions. Second, the generated problems, the assignment instructions, and the corresponding reference solutions are incorporated into a file format that the moodle-based teaching platform can interpret. This file also includes the rules for the correction of student answers. Once uploaded to the moodle-based platform, the pool of automatically generated assignments is ready to use as a moodle STACK question: they can be assigned to tests, randomly distributed to the students, and automatically corrected once students provide their answers. As a result, students get individual exercises and receive direct feedback once they submit their answers. This automated interaction allows students to hand in their assignments several times to improve their work. Thus, mistakes are not “punished” but enable students to learn from them.

We present several examples of problems related to statics, strength of materials, dynamics, and hydromechanics, which have been realized with this scalable homework concept, and discuss challenges in the concept’s implementation.

Mechanics goes data - between opportunities and overload

Wessels, Henning *(TU Braunschweig, Germany)* 15:10

The growing importance of methodological and application competencies in the field of artificial intelligence (AI) cannot be overestimated. Across disciplines, AI is boosting innovative applications and products. Prominent AI approaches have been developed in the context of applications where data is almost endless, e.g. in speech and pattern recognition. In computational modeling however, even with an ever increasing amount of sensor data, data remains limited. More than that, limited access to information by sensing is the ultimate reason for computational modeling. In the context of computational mechanics, data-driven mechanics has become an emerging research area. In terms of education, this poses a challenge. In computational mechanics, AI cannot be regarded as an alternative approach to former tools, but rather as an additional competence that students need to acquire. Thus, didactic concepts are required that do not let students experience AI as an additional math burden, nor as a contemporary toy.

Micro-learning content is particularly suitable here, as a variety of learning formats are possible: from edutainment to virtual laboratory experiments. They also allow for great diversity in terms of the degree of didactisation and can be integrated into blended learning scenarios, for example. This talk addresses recent approaches from the collaborative teaching project KI4All.

MS2: Data-driven computational mechanics

Organizer(s): **de Lorenzis, Laura** *(ETH Zurich)*
Reese, Stefanie *(RWTH Aachen)*
Kästner, Markus *(TU Dresden)*

MS2-01: Data-driven computational mechanics

Date: June 1, 2023 13:30-15:30
Room: HSZ/AUDI

Physics-based and data-driven hybrid modelling of materials, structures and processes.

Chinesta, Francisco *(ENSAM, France)* 13:30
Cueto, Elias *(University of Zaragoza)*

Physics aware digital twins of materials, processes, components and systems enable emulating real assets while ensuring fidelity and efficiency. They embrace physics-based and data-driven functionalities, both enriching mutually. Both should proceed in almost real-time, and the last being able to proceed in the scarce data limit. When applied to materials and processes, model order reduction technologies enable the construction of the so-called surrogate model, whereas data-driven modelling, based in advanced machine learning and artificial intelligence technologies, must be informed by the physics to encompass rapidity and accuracy, in the low data limit. This hybrid approach allows improving accuracy of existing models, as well as constructing models when the existing ones remains too poor or uncertain. Moreover, this setting allows to speed-up predictions, enabling real-time control, decision-making as well as the exploration of the whole design space, crucial in the design of materials and components.

Application of hybrid machine learning approaches to exploit process-structure-property linkages in technological production processes

Klusemann, Benjamin *(1 Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany, ; 2 Institute of Institute for Production Technology and Systems, Leuphana University Lüneburg, 21335 Lüneburg, Germany)* 14:10
Bock, Frederic E. *(1 Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany,)*
Huber, Norbert *(1 Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, 21502 Geesthacht, Germany,)*

In the last years, there has been a strong effort in the development of machine learning models to exploit process-structure-property linkages for different processes of interest. Often, these approaches are based on data only, which creates the need for unreasonable large data sets that are very expensive or even impossible to collect experimentally. Furthermore, well-known physical laws might be neglected within this approach. However, in the last decades, sophisticated models and physical relationships have been extensively developed and could be further used to enhance the developed machine learning models.

In this work, the application of different types of hybrid machine learning approaches will be presented for different technological production processes. For instance, an example of physical feature engineering to improve the prediction of the mechanical properties will be provided. Moreover, an example of hybrid modelling via machine learning correction of physical model output will be shown for residual stress prediction. The last example focusses on a simulation-assisted machine learning approach for the prediction of the final geometry during the solid state friction surfacing process.

What data-driven mechanics can do for structural health monitoring

Wessels, Henning *(Institute for Computational Modeling in Civil Engineering, TU Braunschweig, Germany)* 14:30

Computational models have achieved a high level of accuracy in many applications. However, increased accuracy often comes along with increased complexity and also with increased computational cost. As a consequence, the usage of sophisticated models is often restricted to the design phase of products and infrastructures. Recently, the paradigm of the digital twin, which calls for accurate modelling not only during the design phase but over the entire service life, has received much attention. Models, that need to provide information during service life are often subject to severe time constraints. Thus, digital twins rely on the best possible model that makes predictions within the shortest possible time. Data-driven modeling promises to partially resolve the above described conflict of aims. It enables to use the knowledge embedded in complex computational models not only for the design of materials, structures and products, but increasingly also for their monitoring during service life. In this context, this talk will discuss (1) approaches to parameter identification and inverse problems with physics-informed neural networks and (2) a statistical finite element formulation for displacement and stress inference. It will be demonstrated, that structural health monitoring can be regarded as a computational multi-scale problem.

Data-driven finite element computation of microstructured materials

Weinberg, Kerstin *(Universität Siegen, Germany)* 14:50

In the data-driven finite element analysis the constitutive material modeling is eluded and instead data are directly employed as an input for computational analysis. This model-free description allows to implement arbitrary constitutive relations. It can be especially beneficial when you want to easily change the microstructural material design avoiding to start a new fitting process every time you make a change. Our contribution focuses on the question of how we can use the data-driven finite element analysis for cellular materials. Since experimental data acquisition can be tedious, we suggest using numerical computations of representative volumes. In that way, the micromechanical behavior of the material can be employed to deduce homogenized data points. Here we focus on the modeling of polyurethane foam. Dependent on the manufacturing process and the composition of the constituents, the material properties such as density, pore distribution, and structure of the material vary. To avoid fitting a material model for every case, we use stochastic representative volume elements (RVEs) to generate the data basis. A foam generator produces the RVEs with the desired properties

which are then subjected to some test loads to deduce homogenized data points. To not simulate each point individually, the database is constructed with the help of material properties such as linearity or isotropy. For illustration, the database is used in a finite element computation of a rubber sealing.

Physics-enhanced neural networks for multiscale and multiphysics material modeling

Weeger, Oliver *(TU Darmstadt, Germany)* 15:10
Klein, Dominik K. *(TU Darmstadt, Germany)*
Fernández, Mauricio *(ACCESS e.V., Aachen, Germany)*
Ortigosa, Rogelio *(TU Cartagena, Spain)*

The emergence of advanced and additive manufacturing technologies enables the fabrication of microstructured, architected, and functionally graded materials, which allows the realization of parts with tailored mechanical and multi-functional behaviors. However, to exploit this unprecedented design freedom in engineering applications, accurate computational modeling and design methods are required, which can efficiently consider the complex nonlinear, inelastic, scale-bridging, and multiphysical effects of such metamaterials.

To address this challenge, in this talk we present the development of physics-enhanced neural network constitutive models for hyperelasticity and electro-elasticity at finite deformations. These approaches combine the flexibility of machine learning with a rigorous fulfillment of essential continuum mechanical requirements, such as the laws of thermodynamics, objectivity, material symmetry, growth and normalization conditions, as well as ellipticity. In particular, the latter condition is ensured by developing polyconvex models based on input convex neural networks, which can be formulated either in terms of suitable invariants or directly using the deformation gradient [1,2].

We demonstrate the application of physics-enhanced neural network material models to the nonlinear multiscale modeling of beam lattices [1,3,4], including dependencies on microstructural design parameters [5], as well as to electro-elastic composite materials [2]. These results show that augmenting machine learning with physical requirements greatly improves the accuracy and generalizability of the models while reducing the required amount of training data and providing the necessary flexibility required by complex microstructural behaviors.

References:

[1] https://doi.org/10.1016/j.jmps.2021.104703
[2] https://doi.org/10.1016/j.cma.2022.115501
[3] https://doi.org/10.1007/s00466-020-01954-7
[4] https://doi.org/10.1007/s00466-021-02061-x
[5] https://doi.org/10.1002/nme.6869

MS3: High-order and Parallel Time Integration

Organizer(s): **Götschel, Sebastian** *(TU Hamburg)*
Stiller, Jörg *(TU Dresden)*

MS3-01: High-order and Parallel Time Integration

Date: June 1, 2023 13:30-15:30
Room: HSZ/H03

Parallel-in-time high-order multiderivative IMEX solvers

Schütz, Jochen *(UHasselt, Belgium)* 13:30
Thenery Manikantan, Arjun *(UHasselt, Belgium)*
Theodosiou, Eleni *(UHasselt, Belgium)*
Zeifang, Jonas *(UHasselt, Belgium)*

In this talk, we present recent developments on high-order multiderivative IMEX time integration schemes, with a focus on their use in computational fluid dynamics. First, we present the algorithm for initial-value problems in its predictor-corrector version. This predictor-corrector formulation has some peculiar advantages, in particular, the method can be formulated as a parallel-in-time method. We shortly touch upon the behavior of the method for singularly perturbed equations and show that the resulting algorithm is asymptotically consistent. In a second part, we apply the time integration procedure to the compressible Navier-Stokes equations. The underlying spatial discretization is the discontinuous Galerkin spectral element method (DGSEM). The focus here is on the behavior of the algorithm in a time-parallel environment. It is demonstrated that a suitable load balancing requires an adaptive Newton criterion both over the stages of the method and over the corrector steps. Numerical results are shown, comparing against more established time integrator schemes.

Enhancing scalability through parallel-in-time algorithms using performance modeling

Hahne, Jens *(Bergische Universität Wuppertal, Germany)* 13:50
Friedhoff, Stephanie *(Bergische Universität Wuppertal, Germany)*
Bolten, Matthias *(Bergische Universität Wuppertal, Germany)*

Parallel-in-Time (PinT) methods are a promising approach to reduce simulation times of time-dependent PDEs on modern high-performance computers by introducing parallelism in the temporal dimension. One approach to improve the performance and efficiency of these methods for future exascale HPC systems is to develop load-balancing strategies that respond to load imbalances that may arise, for example, through fault-tolerance mechanisms or by coupling PinT methods with adaptive space-time schemes. A first step in developing such strategies is to develop a performance model to predict the runtimes for different PinT methods, which can later be used to compare different load-balancing strategies.

In this talk, we present a task graph-based performance analysis for iterative PinT methods. In particular, this approach allows for a scheduling-based runtime analysis of the methods, covering their large parameter spaces. Further, we present how this task view of PinT algorithms can be used to improve scalability of the methods.

Across-the-method parallelization of spectral deferred corrections for shallow water equations

Fregin, Joscha *(Hamburg University of Technology, Germany)* 14:10
Lunet, Thibaut *(Hamburg University of Technology, Germany)*
Ruprecht, Daniel *(Hamburg University of Technology, Germany)*
Goetschel, Sebastian *(Hamburg University of Technology, Germany)*

Spectral deferred corrections (SDC) provide an efficient iterative way to solve the fully coupled nonlinear system that arises for fully implicit collocation methods of Runge-Kutta type. SDC can be understood as a Richardson or discrete Picard iteration that uses a low-order method like Euler as a "preconditioner". The choice of preconditioner offers many opportunities to build bespoke methods, e.g. high order implicit-explicit methods. Using a method that corresponds to a diagonal matrix as preconditioner allows to perform some of the computations necessary for a time step in parallel, thus speeding up the method. Optimization can be employed to find good parameters that balance rapid convergence and stability. In our talk, we will present the parallel SDC method, describe results from the parameter optimization. We will assess performance of the resulting algorithm for the Galeswky test problem, simulating the evolution of a barotropic instability on the sphere, using the Dedalus software.

Theoretical and Practical Aspects of Implementations of Space-Time DG-SEM

Versbach, Lea *(Lund University, Sweden)* 14:30
Linders, Viktor *(Lund University, Sweden)*
Klöfkorn, Robert *(Lund University, Sweden)*
Birken, Philipp *(Lund University, Sweden)*
Gassner, Gregor *(University of Cologne, Germany)*

We consider space-time discontinuous Galerkin spectral element methods (DG-SEM) for convection dominated problems. In particular, we compare two archetypical implementation approaches, both of which allow for easy parallelization in time. In one, time is treated as an additional coordinate direction and a Galerkin procedure is applied to the entire problem. In the other, the method of lines is used with DG-SEM in space and the fully implicit Runge-Kutta method Lobatto IIIC in time. The two approaches are mathematically equivalent in the sense that they lead to the same discrete solution. However, in practice they differ in several important respects, including the terminology used to describe them, the structure of the resulting software, and the interaction with nonlinear solvers. Challenges and merits of the two approaches are discussed with the goal of providing the practitioner with sufficient consideration to choose which path to follow. A particular focus is put on iterative solvers, such as multigrid methods. Additionally, implementations of the two methods in the open source

DUNE framework are presented as a starting point for further development. Numerical experiments validate the theoretical accuracy of these codes and demonstrate their utility, even for 4D problems.

Parallel-in-Time Integration of Transients in Superconducting Accelerator Magnets

Schnaubelt, Erik *(CERN, Switzerland; Technical University of Darmstadt, Germany)* 14:50
Wozniak, Mariusz *(CERN, Switzerland)*
Dular, Julien *(University of Liège, Belgium)*
Cortes Garcia, Idoia *(Eindhoven University of Technology, Netherlands)*
Schöps, Sebastian *(Technical University of Darmstadt, Germany)*

Superconducting accelerator magnets generate high magnetic fields to steer the particle beam with relatively low energy consumption. Local transition to a normal-conducting state due to, e.g., local heat generation can lead to a thermal run-away called quench. Numerical tools such as the finite element method are crucial to understand the transient behaviour of superconducting magnets. These quench simulations are intrinsically multi-physics problems involving coupled electromagnetism, thermodynamics, and, eventually, solid mechanics. As a local, transient phenomenon, quench generally requires three-dimensional simulation in time with high number of degrees of freedom. Furthermore, as material properties over a wide temperature range must be considered, the problem is highly non-linear. For this reason, it typically requires small time steps over a large time interval to capture the thermal run-away properly. To mitigate these challenges, we discuss parallel-in-time methods for quench simulation of superconducting accelerator magnets.

Acknowledgment. The work of Erik Schnaubelt has been sponsored by the Wolfgang Gentner Programme of the German Federal Ministry of Education and Research (grant no. 13E1-8CHA) and by the Graduate School Computational Engineering within the Centre for Computational Engineering at the Technical University of Darmstadt.

IMEX Runge-Kutta and Spectral Deferred Correction Methods for Incompressible Navier-Stokes Problems

Stiller, Jörg *(TU Dresden, Germany)* 15:10

When performing flow simulations using high-order spatial discretization methods, such as DG-SEM, it is natural to use a high-order method in time as well. In this talk, we consider Runge-Kutta and spectral deferred correction (SDC) methods for incompressible Navier-Stokes problems with constant or variable viscosity.

The following questions are addressed:

1) How to construct these methods based on implicit-explicit splitting schemes?
2) What order reduction is observed with unsteady boundary conditions or variable viscosity?
3) How do these methods compete with popular multistep methods such as BDF2?
4) What can be achieved by getting more implicit?

MS4: Data-driven Methods in Systems and Control

Organizer(s): **Faulwasser, Timm** *(TU Dortmund)*
Heiland, Jan *(MPI Magdeburg)*
Worthmann, Karl *(TU Ilmenau)*

MS4-01: Data-driven Methods in Systems and Control

Date: June 1, 2023 13:30-15:30
Room: HSZ/H04

Multi-classification using Deep Neural Networks

Zuazua, Enrique *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; Universidad Autónoma de Madrid, Spain)* 13:30
Hernandez, Martin *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*

We analyze the multi-classification problem for a d-dimensional data set with N elements and M classes. We consider a multilayer perceptron in the non-residual case, so it is not possible to interpret this architecture as a so-called neural ordinary differential equation. We prove that this deep neural network with a depth of 2N+4M+1 can solve the classification problem. The proof is based on a geometrical interpretation of the neural network, allowing us to train the neural network in a constructive way. That is, the parameters are constructed inductively and explicitly without solving any minimization problem. To keep the geometrical interpretations and to perform a simple and systematic proof, the d-dimensional data are carried into a two-dimensional space to be treated. Therefore, each hidden layer of the network has at most two neurons, thus being the architecture of a narrow neural network.

The constructive procedure for training the neural network is done in four steps. The first hidden layer is in charge of the preconditioning of the data, in which we project them in a one-dimensional space. Then, we perform a compression procedure in which, using 2N layers, the data from the same class are compressed into one single point. Afterward, 5+2(M-1) layers are responsible for sorting the data in increasing order according to their labels. Finally, we map the data to their respective labels using 1+2(M-2) layers.

Data-driven Control and Behaviors of Stochastic Systems – Combining the Ideas of Wiener and Willems

Faulwasser, Timm *(TU Dortmund, Germany)* 13:50
Ou, Ruchuan *(TU Dortmund, Germany)*
Pan, Guanru *(TU Dortmund, Germany)*
Schmitz, Philipp *(TU Ilmenau, Germany)*
Worthmann, Karl *(TU Ilmenau, Germany)*

There are manifold recent research efforts on data-driven control based on the fundamental lemma by Jan C. Willems and co-authors [1]. The lemma as such states that the finite-horizon behavior of any controllable discrete-time LTI system can be characterised by the image of Hankel matrices constructed from suitable input-state-output trajectory data.

In this talk we recapitulate on our recent efforts towards a stochastic extension of Willems' lemma [2,3]. We leverage polynomial chaos expansions of L^2 random variables - which date

back to foundational contributions of Norbert Wienerand which are frequently used for uncertainty quantification [4,5] - to represent non-Gaussian and Gaussian uncertainty in a linear fashion. Combining the linearity of the series expansion with the linear system structure we construct a stochastic extension of the fundamental lemma. Moreover, we show how this lemma paves the road towards the characterization of the behavior of stochastic linear systems in terms of random variables and in terms PCE coefficients. We explore the relations of these behaviours to the path-wise perspective of sampled realisation trajectories. The talk concludes with numerical examples and with an outlook on open problems.

[1] Willems, Jan C., Paolo Rapisarda, Ivan Markovsky, and Bart LM De Moor. "A note on persistency of excitation." *Systems & Control Letters* 54, no. 4 (2005): 325-329.
[2] Pan, Guanru, Ruchuan Ou, and Timm Faulwasser. "On a stochastic fundamental lemma and its use for data-driven optimal control." *IEEE Transactions on Automatic Control* (2022).
[3] Faulwasser, Timm, Ruchuan Ou, Guanru Pan, Philipp Schmitz, and Karl Worthmann. "Behavioral theory for stochastic systems? A data-driven journey from Willems to Wiener and back again." arXiv preprint `https://arxiv.org/abs/2209.06414` (2022).
[4] Wiener, Norbert. "The homogeneous chaos." *American Journal of Mathematics* 60, no. 4 (1938): 897-936.
[5] Sullivan, Timothy John. *Introduction to uncertainty quantification*. Vol. 63. Springer, 2015.

On reliable data-based predictive control in the Koopman framework

Nüske, Feliks *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany)*
Peitz, Sebastian *(Paderborn University, Department of Computer Science, Data Science for Engineering, Germany)*
Philipp, Friedrich *(Technische Universität Ilmenau, Institute of Mathematics, Optimization-based Control group, Germany)*
Schaller, Manuel *(Technische Universität Ilmenau, Institute of Mathematics, Optimization-based Control group, Germany)*
Worthmann, Karl *(Technische Universität Ilmenau, Institute of Mathematics, Optimization-based Control group, Germany)*

14:10

Extended Dynamic Mode Decomposition, embedded in the Koopman framework, is a widely-applied technique to predict the evolution of an observable along the flow of a dynamical control system. However, despite its popularity, the error analysis is still fragmentary. We provide a complete and rigorous analysis for control-affine systems by splitting up the approximation error into the projection and estimation error resulting from the finite dictionary size [3] and the finite amount of i.i.d. data used to generate the surrogate model [1]. If time permits, an extension towards reproducible kernel Hilber spaces is indicated, see [2] for details.

Then, the usefullness of the derived surrogate model for predictive control is demonstrated and discussed.

References

[1] Feliks Nüske, Sebastian Peitz, Friedrich Philipp, Manuel Schaller, and Karl Worthmann. Finite-data error bounds for Koopman-based prediction and control. Journal of Nonlinear Science, 33:14, 2023.

[2] Friedrich Philipp, Manuel Schaller, Karl Worthmann, Sebastian Peitz, and Feliks Nüske. Error bounds for kernel-based approximations of the koopman operator. 2023. arXiv preprint https://arxiv.org/abs/2301.08637.
[3] Manuel Schaller, Karl Worthmann, Friedrich Philipp, Sebastian Peitz, and Feliks Nüske. Towards reliable data-based optimal and predictive control using extended DMD. In Proc. 12th IFAC Symposium on Nonlinear Control Systems, IFAC-PapersOnLine, to appear, arXiv preprint https://arxiv.org/abs/2202.09084.

Subsampling in ensemble Kalman inversion

Hanu, Matei *(Free University Berlin, Germany)*
Latz, Jonas *(Heriot-Watt University)*
Schillings, Claudia *(Free University Berlin, Germany)*

14:30

We consider the ensemble Kalman inversion which has been recently introduced as an efficient, gradient-free optimisation method to estimate unknown parameters in an inverse setting. In the case of large data sets, the ensemble Kalman inversion becomes computationally infeasible as the data misfit needs to be evaluated for each particle in each iteration. Here, randomised algorithms like stochastic gradient descent have been demonstrated to successfully overcome this issue by using only a random subset of the data in each iteration, so-called subsampling techniques. Based on a recent analysis of a continuous-time representation of stochastic gradient methods, we propose, analyse, and apply subsampling-techniques within ensemble Kalman inversion. Indeed, we propose two different subsampling techniques: either every particle observes the same data subset (single subsampling) or every particle observes a different data subset (batch subsampling).

Gaussian Process-Based Online Learning for Control with Performance Guarantees

Lederer, Armin *(Technical University of Munich, Germany)*
Hirche, Sandra *(Technical University of Munich, Germany)*

14:50

In many real-world applications, the system models employed in control are unknown or merely partially known, e.g, due to complex environmental effects found in underwater robotics, or the lack of first principle models in human-robot interaction. In order to achieve a high control performance despite this model inaccuracy, supervised machine learning is commonly employed to improve the model precision. In this talk, we focus on Gaussian process regression for inferring a model of the system dynamics due to the existence of statistical prediction error bounds. These error bounds admit a pessimistic analysis of the control performance, which we exemplarily demonstrate by deriving a tracking error bound for linear systems with unknown input perturbation. Due to the strong dependency of these results on the model uncertainty, we can show that arbitrarily small tracking errors can be guaranteed by updating the Gaussian process model online with a sufficiently high frequency. In order to achieve high model update rates, we propose a computationally efficient approximation for Gaussian process regression based on a local model aggregation. Since the proposed approximation maintains relevant theoretical guarantees of exact Gaussian process regression, performance

guarantees for control directly extend to it. Finally, the practical applicability of the proposed approach is demonstrated in a human-robot interaction experiment.

Data-driven Robust Model Predictive Control exploiting Finisler's Lemma and LMI Reformulations

Nguyen, Hoang Hai *(TU Darmstadt, Control and Cyber-Physical Systems Laboratory, Germany)* 15:10

Friedel, Maurice *(TU Darmstadt, Control and Cyber-Physical Systems Laboratory, Germany)*

Findeisen, Rolf *(TU Darmstadt, Control and Cyber-Physical Systems Laboratory, Germany)*

Predictive Control is widely used to optimize the future behavior of a system by utilizing a system model to determine the optimal input. However, when nominal models are not available or are unreliable, data-driven model predictive control methods can be utilized by directly obtaining the system model or input from past measured trajectories. We propose a robust data-driven model predictive control scheme that considers both input and state constraints. The scheme is based on a linear matrix inequality approach, which utilizes Finsler's lemma and a data informativity framework. We consider two cases: slowly varying linear systems and Lur'e systems with uncertain nonlinearity. Our approach formulates the problem as a semi-definite optimization problem, which provides the matrix gain for the linear feedback. This method is independent of the length of the measurement data, making it suitable for larger data sets. Our designed controller stabilizes the closed-loop system asymptotically and ensures that the constraints are satisfied.

MS5: Port-Hamiltonian systems

Organizer(s): **Jacob, Birgit** *(Bergische Universität Wuppertal)*
Kotyczka, Paul *(TU München)*

MS5-01: Port-Hamiltonian systems

Date: June 1, 2023 13:30-15:30
Room: CHE/S89

Boundary controlled Oseen equations in port-Hamiltonian formulation

Reis, Timo *(TU Ilmenau, Germany)* 13:30
Schaller, Manuel *(TU Ilmenau, Germany)*

We consider Oseen equations, i.e., Navier-Stokes equations which are linearized around a steady state. First we discuss classical boundary conditions for this type, such as velocity prescription, no-slip or "do-nothing" conditions. Thereafter, we present a port-Hamiltonian formulation of boundary-controlled Oseen equations. Our formulation will be on the basis of the framework on so-called "system nodes" by O. Staffans. As a benchmark example, we discuss a pipeline with in- and outflow.

Differential-algebraic systems with dissipative Hamiltonian and maximally monotone structure

Mehrmann, Volker *(TU Berlin, Germany)* 13:50
van der Schaft, Arjan *(University of Groningen, The Netherlands)*

Different representations of linear Hamiltonian differential-algebraic equations (DAE) systems are presented and compared. Using global geometric and algebraic points of view, translations between the different representations are presented. Characterizations are also derived when a general DAE system can be transformed into one of these structured representations. Approaches for computing the structural information and the described transformations are presented that can be directly implemented as numerical methods. The results are extended to maximally monotone structures and it is shown that any such structure can be written as decomposition of a Dirac and a resistive structure. Furthermore, appropriate coordinate representations are presented as well as explicit expressions for the associated transfer functions.The results are demonstrated with a large number of examples.

Don't forget the energy: model reduction for port-Hamiltonian systems

Nicodemus, Jonas *(Universität Stuttgart, Germany)* 14:10
Schwerdtner, Paul *(Technische Universität Berlin)*
Unger, Benjamin *(Universität Stuttgart, Germany)*

It is well known that any port-Hamiltonian (pH) system is passive, and conversely, any minimal and stable passive system has a pH representation. Nevertheless, this equivalence is only concerned with the input-output mapping but not with the Hamiltonian itself. Thus, we propose to view a pH system as either an enlarged dynamical system with the Hamiltonian as additional output or as two dynamical systems. We study the effect of this viewpoint on the

observability of the system and discuss implications for optimal model reduction, which can be recast as a dual-objective optimization problem. We discuss certain aspects of the Pareto front and provide numerical exampels for further insights.

Nonlinear elastodynamics in the context of port-Hamiltonian modeling: Formulation and structure-preserving discretization

Kinon, Philipp Lothar *(Karlsruhe Institute of Technology (KIT), Germany)* 14:30
Thoma, Tobias *(Technical University of Munich (TUM), Germany)*
Betsch, Peter *(Karlsruhe Institute of Technology (KIT), Germany)*
Kotyczka, Paul *(Technical University of Munich (TUM), Germany)*

Port-Hamiltonian (PH) systems provide a framework for modeling, analysis and control of complex dynamical systems, where the complexity might result from multi-physical couplings, non-trivial domains and diverse nonlinearities. A major benefit of the PH representation is the explicit formulation of power interfaces, so-called ports, which allows for a power-preserving interconnection of subsystems. Thus, models can be easily composed in a modular way. Accordingly, models from various physical disciplines have already been transferred into a PH representation. In the context of structural mechanics, however, nonlinear PH models remain an exception and most contributions account for linear systems only.

We present a PH formulation for hyperelastic mechanical systems with a nonlinear stored energy function together with a suitable structure-preserving discretization. We motivate the approach by considering the nonlinear elastic spring pendulum, which represents a well-known model problem in the field of structural elastodynamics. However, the formulation can also be applied to infinite-dimensional systems, such as strings or beams. In this case, using a mixed finite element method achieves a spatial discretization, which retains the ports (e.g., pairs of velocities and forces) on the discrete level. Moreover, the temporal discretization makes use of discrete derivatives in the sense of Gonzalez and yields an energy-momentum consistent time-stepping scheme.

Additionally, the discrete PH state space model might be used for feedforward or feedback control design (which are not in the focus of this contribution). The numerical properties of the devised formulation are investigated in more detail in a representative example.

References:

V. Duindam, A. Macchelli, S. Stramigioli, H. Bruyninckx: Modeling and Control of Complex Physical Systems, Springer Berlin Heidelberg (2009).
T. Thoma, P. Kotyczka: Port-Hamiltonian FE models for filaments, IFACPapersOnLine 55.30: 353-358 (2022).
O. Gonzalez: Time integration and discrete Hamiltonian systems, J. Nonlinear Sci. 6: 449-467 (1996).

Optimal Control of Port-Hamiltonian Systems – Putting Energy in the Objective

Faulwasser, Timm *(TU Dortmund, Germany)* 14:50
Maschke, Bernhard *(Université Lyon 1, France)*
Philipp, Friedrich *(TU Ilmenau, Germany)*
Schaller, Manuel *(TU Ilmenau, Germany)*
Worthmann, Karl *(TU Ilmenau, Germany)*

Hamiltonian structures are of fundamental importance in the calculus of variations and in optimal control theory. As such, they are inherently present in the optimality system, i.e., they arise from optimality considerations and from the Lagrangian formalism which adjoins the dynamics to the objective functional. Hence, the question of how port-Hamiltonian (pH) structures can be exploited in the analysis and in the numerical solution of optimal control problems is intuitive - yet it is also far from being conclusively resolved.

In this talk, we provide first answers and insights. We show that the pH structure becomes particularly relevant if the considered objective also reflects the pH structure. That is, we consider the problem of minimizing the energy supplied to a pH system under additional constraints [1,2]. We show that - while exhibiting singular arcs - for this class of problems the pH structure induces favourable structure to the optimality system [1]. We discuss recent results for differential algebraic systems and for nonlinear pH structures arising from thermodynamical systems [2,3]. Our findings are closely linked to the turnpike phenomenon in optimal control, i.e., the phenomenon that for varying initial conditions and horizon length the optimal solutions stay close to the infinite-horizon optimal attractor [4]. We introduce the concepts manifold and subspace turnpike properties to characterise the solution structure [1,5]. We draw upon examples from thermodynamics and mechanics to illustrate our findings.

[1] Schaller, Manuel, Friedrich Philipp, Timm Faulwasser, Karl Worthmann, and Bernhard Maschke. “Control of port-Hamiltonian systems with minimal energy supply.” *European Journal of Control* 62 (2021): 33-40.
[2] Faulwasser, Timm, Bernhard Maschke, Friedrich Philipp, Manuel Schaller, and Karl Worthmann. “Optimal control of port-Hamiltonian descriptor systems with minimal energy supply.” *SIAM Journal on Control and Optimization* 60, no. 4 (2022): 2132-2158.
[3] Maschke, Bernhard, Friedrich Philipp, Manuel Schaller, Karl Worthmann, and Timm Faulwasser. “Optimal control of thermodynamic port-Hamiltonian systems.” *IFAC-PapersOnLine* 55, no. 30 (2022): 55-60.
[4] Faulwasser, T., and L. Grüne. “Turnpike properties in optimal control.” *Handbook of Numerical Analysis* 23 (2022): 367-400.
[5] Faulwasser, Timm, Kathrin Flaßkamp, Sina Ober-Blöbaum, Manuel Schaller, and Karl Worthmann. “Manifold turnpikes, trims, and symmetries.” *Mathematics of Control, Signals, and Systems* 34, no. 4 (2022): 759-788.

Structure-Preserving Methods for a Coupled port-Hamiltonian System of Compressible Non-Isothermal Fluid Flow

Hauschild, Sarah-Alexa *(Universität Trier, Germany)*
Marheineke, Nicole *(Universität Trier, Germany)*

15:10

The port-Hamiltonian formulation of partial-differential equations and their numerical treatment have been elaborately studied lately. One advantage of port-Hamiltonian systems is that fundamental physical properties, like energy dissipation and mass conservation, are encoded in the system structure. Therefore, structure-preservation is most important during all stages of approximation and system coupling. In this context we consider the non-isothermal flow of a compressible fluid through a network of pipes. Based on a port-Hamiltonian formulation of Euler-type equations on one pipe, we introduce coupling conditions, through which we can realize energy, mass and entropy conservation at the coupling nodes and thus, preserve the port-Hamiltonian structure. We implement them through an input-output-coupling using the flow and effort variables of the boundary port of the underlying Dirac structure. Thus, we can make use of the structure-preserving model and complexity reduction techniques for the single pipe. This procedure becomes even more important for network simulations, as here, we deal with high dimensional and highly non-linear dynamical systems. We explain the extension from a single pipe to a network and numerical examples are shown to support our findings.

MS6: Modelling and simulation of thin mechanical films

Organizer(s): **Bartels, Sören** *(Universität Freiburg)*
Neukamm, Stefan *(TU Dresden)*
Sander, Oliver *(TU Dresden)*

MS6-01: Modelling and simulation of thin mechanical films

Date: June 1, 2023 13:30-15:30
Room: POT/51

Effective models for membranes and plates with soft inclusions

Schmidt, Bernd *(Universität Augsburg, Germany)* 13:30

We report on some recent results on effective theories for thin and ultrathin films which are subject to both elastic deformations and fracture. In particular, we will consider the formation of voids and cracks in membranes and Kirchhoff plates. (Joint work with M. Santilli, l'Aquila.)

Simulating models for nonlinear plate bending

Palus, Christian *(Albert-Ludwigs-Universität Freiburg, Germany)* 14:00

When thin mechanical films are modelled a typical approach is to investigate the limiting case of vanishing thickness. However, resulting two-dimensional models can still be complex, thus making it hard to develop an intuitive understanding of the mechanical behaviour without the help of reliable numerical simulations. In the talk we propose a numerical method based on a discrete gradient flow of the model energy for approximating nonlinear plate bending models. The use of discrete Kirchhoff elements for discretizing corresponding deformations allows for the prescription of metric constraints at the nodes of a triangulation. We present numerical simulations demonstrating how the method can be applied to better understand the mechanical behavior of a two-dimensional model of nematic liquid crystal elastomer plates.

Amplitude expansion of the phase-field crystal model on deformable surfaces

Benoit–Maréchal, Lucas *(Institute of Scientific Computing, TU Dresden, Dresden, Germany)* 14:30
Salvalaglio, Marco *(Institute of Scientific Computing, TU Dresden, Dresden, Germany)*
Nitschke, Ingo *(Institute of Scientific Computing, TU Dresden, Dresden, Germany)*
Voigt, Axel *(Institute of Scientific Computing, TU Dresden, Dresden, Germany)*

The Phase Field Crystal (PFC) model describes lattices at diffusive timescales but atomic length-scales, thus requiring subatomic resolution meshes. To remedy this restriction, the complex amplitude expansion (APFC) was developed, whereby the amplitude of the density fluctuations is modeled instead of the density itself, enabling simulations at mesoscales that retain atomistic features. We extend the two-dimensional APFC model to include out-of-plane displacements in order to study the coupling between crystal defects and surface deformation, paving the way for applications such as the topological tuning of mechanical properties of crystalline sheets. To validate our model, we compare representative settings with atomistic

simulations from the PFC model and Molecular Dynamics and find, within certain limits that we discuss, excellent agreement between all models.

Dimension reduction and homogenization for fluid flow across a thin porous elastic layer

Gahn, Markus *(University of Heidelberg, Germany)* 15:00
Jäger, Willi *(University of Heidelberg, Germany)*
Neuss-Radu, Maria *(Friedrich-Alexander-University Erlangen-Nuremberg, Germany)*

In this talk we derive a coupled Stokes-plate model for fluid flow across a thin porous elastic layer, which separates two fluid-filled bulk domains. The thin periodically perforated layer consists of a fluid and an elastic solid part. Thickness and periodicity of the layer are of order ϵ, where the parameter ϵ is small compared to the size of the bulk domains. The evolution of the fluid flow is described by an instationary Stokes system, and the solid via linear elasticity. At the fluid-solid interface we assume a linearized coupling condition for the velocities and the stresses. We proceed a simultaneous homogenization and dimension reduction to derive a macroscopic model with effective interface laws and homogenized coefficients for ϵ to 0, when the thin layer reduces to an interface Σ separating the two bulk domains. To pass to the limit ϵ to 0 we use multi-scale techniques adapted to problems in continuum mechanics, including extension operators for perforated domains preserving ϵ-uniform bounds for the symmetric gradient, Korn-inequalities, and two-scale compactness of ϵ-dependent sets in Sobolev spaces on thin perforated layers. We show that the effective model consists of the instationary Stokes equations in the bulk domains coupled to a time dependent plate equation on the interface Σ including homogenized elasticity coefficients carrying information about the micro structure of the layer. The macroscopic fluid velocity is continuous at the interface, where only a vertical movement occurs and the tangential components vanish. The macroscopic displacement is given as a Kirchhoff-Love displacement.

Young Researchers' Minisymposia

YRM1: Randomized algorithms in numerical linear algebra

Organizer(s): **Cortinovis, Alice** *(École Polytechnique Fédérale de Lausanne)*
Boullé, Nicolas *(University of Oxford)*

YRM1-01: Randomized algorithms in numerical linear algebra

Date: May 30, 2023 16:30-18:30
Room: HSZ/H03

Randomized Joint Diagonalization of Symmetric Matrices

He, Haoze *(École Polytechnique Fédérale de Lausanne (EPFL))* 16:30
Kressner, Daniel *(École Polytechnique Fédérale de Lausanne (EPFL))*

A basic linear algebra result states that a family of two or more commuting symmetric matrices has a common eigenvector basis and can thus be jointly diagonalized by an orthognoal transformation. Perhaps surprisingly, the development of a robust numerical algorithm for effecting such a joint diagonalization is by no means trivial. To start with, roundoff error or other forms of error will inevitably destroy the commutativity assumption. In turn, one can at best hope to find an orthogonal transformation that nearly diagonalizes every matrix. Most existing approaches deal with this problem via general, expensive optimization techniques. In this talk, we propose a novel randomized method that addresses the joint diagonalization problem by reducing the joint diagonalization problem to standard eigenvalue problems via random linear combination. Unlike existing optimization-based methods, our algorithm is nearly trivial to implement and leverages existing high-quality linear algebra software packages. We prove robust recovery: With high probability, our algorithm achieves joint diagonalization up to the level of the input error, independent of matrix properties such as eigenvalue gaps. We will discuss an improvement with deflation techniques. Through numerical experiments on synthetic and real-world data, we demonstrate that our algorithm is highly competitive compared to the state-of-the-art.

Randomized Krylov methods for efficient solution of linear systems and eigenvalue problems.

Balabanov, Oleg *(Inria, France)* 16:50
Grigori, Laura *(Inria, France)*

In this talk we integrate the random sketching technique into Krylov methods for the efficient solution of sparse linear systems and eigenvalue problems. The core ingredient of our methodology is the estimation of inner products of high-dimensional vectors by inner products of their small, efficiently computable random images, called sketches. This enables the imposition of orthogonality conditions inherent in Krylov methods by operating on sketches rather than high-dimensional vectors, resulting in significant computational savings. We will present a randomized version of the Arnoldi iteration for constructing a Krylov basis and randomized versions of GMRES and Rayleigh-Ritz methods for obtaining a solution in this basis.

Rigorous guarantees of accuracy and stability of the methods will be established based on the fact that the sketching embedding is, with high probability, an approximate isometry for the Krylov space. The talk will conclude with a discussion of the methodology's potential for modern computational architectures, with a particular focus on s-step Krylov methods.

On the Unreasonable Effectiveness of Single Vector Krylov for Low-Rank Approximation

Meyer, Raphael *(New York University)* 17:10
Musco, Cameron *(University of Massachusetts Amherst)*
Musco, Christopher *(New York University)*

A common task in NLA is low-rank approximation, which can be done by approximating the top eigenvectors of a matrix. Block Krylov Iteration gives the best known theoretical guarantees and empirical performance for this task. Though, it's conceptually unclear how we should choose the block size. The best theoretical guarantees in the prior work requires using large block sizes, at least block size k when finding a rank-k approximation – and possibly much larger. However, in practice, a small constant block size independent of k typically performs much better than such large block sizes. When the block size is exactly 1, we call this "Single Vector Krylov". We resolve this unclarity and this theory-practice gap by proving that, when counting matrix-vector products instead of iteration complexity, Single Vector Krylov matches the rate of convergence of the best possible choice of block size, up to just a mild logarithmic dependence on eigenvalue gaps. Moreover, for a wide family of matrices, Single Vector Krylov converges faster, improving from $O(k \cdot \log(1/\epsilon))$ MatVecs to $O(k+\log(1/\epsilon))$ MatVecs. The core of our proof is the observation that the Krylov Subpsace generated by Single Vector Krylov initialized from random vector is exactly equal to the Krylov Subspace generated by Block Krylov Iteration initialized to a structured starting block. We conclude with implications of this theory for simplifying algorithms, smoothed analysis, and experimental validation.

Randomized preconditioning for least squares in mixed precision

Daužickaitė, Ieva *(Charles University, Czech Republic)* 17:30
Carson, Erin Claire *(Charles University, Czech Republic)*

Effective preconditioners for dense least square problems can be obtained via randomized techniques. These require randomly sketching the coefficient matrix to obtain a smaller representation and then computing its deterministic factorisation. The process for generating the preconditioner can be made more efficient by using a mixed precision framework, where different steps of the algorithm are performed in different precisions. Caution is needed when choosing the precisions so that we acquire a final solution of a required accuracy. In this work, we consider a preconditioner coming from a QR factorization of the sketched coefficient matrix. We theoretically analyse how the preconditioner is affected by performing expensive computations in low precisions and illustrate it numerically. Particular attention is paid to using such preconditioner in an iterative refinement setting.

Multigrid Multilevel Monte Carlo and Deflation

Ramirez-Hidalgo, Gustavo *(Bergische Universität Wuppertal, Germany)* 17:50
Frommer, Andreas *(Bergische Universität Wuppertal, Germany)*
Jimenez-Merchan, Jose *(Bergische Universität Wuppertal, Germany)*

In many applications, the trace of a sparse and large matrix needs to be computed. In particular, in lattice quantum chromodynamics (LQCD), the trace of the inverse of the discretized Dirac operator appears in the disconnected fermion loop contribution to an observable. As simulation methods get more and more precise, these contributions become increasingly important. Hence, we consider here the problem of computing the trace $\mathrm{tr}(D^{-1})$, with D the Dirac operator.

The Hutchinson method, which is frequently used to stochastically estimate the trace of the function of a matrix, approximates the trace as the average over estimates of the form $x^H D^{-1} x$. Here, the entries of the vector x follow a certain probability distribution. For N samples, the accuracy for such a Monte Carlo approximation is $O(1/N^{1/2})$.

In recent work, we have introduced multigrid multilevel Monte Carlo: having a multigrid hierarchy with operators A_i, P_i and R_i, for level i, we can rewrite the trace in the form $\mathrm{tr}(A_0^{-1})=\sum_{i=0}^{L-1}\mathrm{tr}(A_i^{-1}-P_iA_{i+1}^{-1}R_i)+\mathrm{tr}(A_L^{-1})$ (this reduced expression is in the special case when $R_iP_i=I$). We can take, in the particular case of LQCD, A_0 to be the Dirac operator D. For some cases, for example the standard 2D Laplacian, we have seen significant reductions in the variance and the total computational work with respect to exactly-deflated Hutchinson.

In this talk, we explore the use of (exact and inexact) deflation in combination with the multigrid multilevel Monte Carlo method, and demonstrate how this leads to both algorithmic and computational gains in comparison with exactly-deflated Hutchinson. Our implementations and tests make use of High Performance Computing, and the results shown are relevant to LQCD.

The parallelization of sketching algorithms for the tensor-train decomposition

Shi, Tianyi *(Lawrence Berkeley National Laboratory, United States of America)* 18:10
Ruth, Maximilian *(Cornell University, United States of America)*
Townsend, Alex *(Cornell University, United States of America)*

In this talk, we propose TT-Sketching, a new parallelizable tensor-train decomposition algorithm for streaming tensor data. We introduce a couple of variants of this algorithm for computation and storage efficiency. For these variants, we provide theoretical guarantees of accuracy, parallel implementation details using message passing interface (MPI), and scaling analysis. Strong scaling results on different tensors suggest that TT-Sketching is better than its serial counterpart, and scales well with the number of computing cores.

YRM2: Novel Modelling Approaches in Structural Stability

Organizer(s): **Köllner, Anton** *(TU Berlin)*
Groh, Rainer *(University of Bristol)*

YRM2-01: Novel Modelling Approaches in Structural Stability

Date: May 30, 2023 16:30-18:30
Room: HSZ/H04

Efficient modelling of nonlinear structural instability problems with material damage

Köllner, Anton *(Technische Universität Berlin, Germany)* 16:30

A novel analytical framework for the inclusion of damaging processes in a structural stability analysis is presented. The work addresses the need for efficient analysis tools in the design of engineering structures that require either the explicit consideration of damage (e.g. damage tolerant design) and/or the full exploitation of the structural strength. As a consequence, structures prone to buckling instability must inevitably also consider material damage and inelasticity. The framework considers quasi-static deformation processes and is formulated in terms of a discrete coordinate approach. A novel energy functional, i.e. an extended total potential energy, is introduced and employed within a variational principle. The inherent complexity of problems involving buckling instability and material damage is made accessible for (semi-)analytical modelling approaches by exploiting the concept of stable damage growth, where equality holds between thermodynamic forces (damage/crack driving forces) and corresponding thresholds. Hence, in the energy functional, the current damage state is expressed in terms of the geometric configuration and the applied loading, such that damage parameters do not explicitly enter the variational statement. However, all characteristic conditions for describing damage growth can also be obtained by the proposed formalism. Owing to the a priori determination of expressions for the damage parameters, the variational problem can be efficiently solved. This allows a systematic analysis of problems in which structures undergo buckling instability and are vulnerable to material damaging. The application of the framework is demonstrated by studying the problem of composite panels with delaminations and matrix cracked layers loaded under in-plane compression.

A Fast Design Tool for Tracing the Geometrically Nonlinear Response of Thin-walled Aircraft Structures

Zucco, Giovanni *(University of Limerick, Ireland)*
Weaver, Paul M *(University of Limerick, Ireland)* 17:00

The geometrically nonlinear behaviour of thin-walled aircraft structures is crucial in the design procedure. Many of these structures exhibit a certain degree of symmetry, which plays an integral role in their elastic post-buckling analysis. This work presents a design tool based on an asymptotic method and a finite element discretisation for tracing the geometrically nonlinear response of elastic thin-walled aircraft structures. In particular, a Koiter-inspired

multi-modal approach that exploits the symmetry properties of a structural system for simplified yet accurate post-buckling analysis is presented. Furthermore, this tool uses a mixed finite element formulation that is derived from the Hellinger-Reisner variational principle.

Firstly, symmetry groups for nonlinear elastic structural systems are discussed in the context of the Group Representation Theory. As such, a general definition for classifying a given structural system's symmetry group is provided based on its geometry's symmetry properties, stiffness distribution, loading and boundary conditions. Then, in the framework of a multi-modal Koiter-inspired theory, we invoke Curie's principle [1]. In this manner, the nonlinear relationship between the symmetry groups of a structural system and related pre-buckling and buckling deformation patterns is exploited to simplify the problem. Then, once the symmetry group of the structural system is detected, we re-invoke Curie's principle for finding the relationship between linear buckling modes and postbuckled deformation of the structure. Subsequently, we furnish a criterion for a priori identification of the set of buckling modes that best describe the post-buckling behaviour of the system under consideration. Then, based on this information, a simplified asymptotic description is obtained by retaining only the subset of the most representative buckling modes in subsequent analysis.

The equilibrium paths obtained with the proposed design tool are compared to benchmark results using the commercial finite element software ABAQUS. Furthermore, insights on the buckling deformation patterns giving the most significant contributions to the asymptotic description of their geometrically nonlinear response are provided.

Numerical results on the geometrically nonlinear behaviour of some primary aircraft structural components under compressive loads obtained with the proposed tool will be presented at the conference. Finally, its computational advantages for tracing the geometrically nonlinear response of thin-walled structures with respect to standard software based on finite element analysis will be commented on.

References

[1] Zucco G. and Weaver P.M.. The role of symmetry in the post-buckling behaviour of structures. 2020: 476(2233). Proc. R. Soc. A.

Multifield computational model predicts the interplay between cellular processes and geometrical instabilities in the developing human brain

Zarzor, Mohammad Saeed *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
Blümcke, Ingmar *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
Budday, Silvia *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*

17:30

During development, the human brain's initially smooth surface evolves into a highly convoluted pattern. The folded morphology correlates with brain function and is thus a valuable marker for neurological disorders. More and more evidence suggests that mechanical instabilities play an important role during the cortical folding process. The precisely orchestrated cellular mechanisms during brain development lead to differential growth between different layers, inducing primary and secondary geometrical instabilities. Understanding the complex interplay between cell behavior and the characteristically folded surface morphology of the human brain is key to better understand, diagnose, and treat diseases associated with malformations of cortical development.

Here, we present a multifield computational framework, which couples an advection-diffusion model describing cell division, migration, and diffusion with the theory of finite growth to capture associated volume growth and cortical folding. We validate our model based on histologically stained sections of human fetal brains and study the effect of different coupling mechanisms between cellular processes and cortical folding in 2D and 3D. The proposed model successfully mimics the evolution of the cell density and folding morphology in the developing human brain. Our results further highlight how primary and secondary geometrical instabilities control the complexity of the evolving cortical folding pattern. The presented framework not only improves our understanding of human brain development, but could eventually help diagnose and treat neurological disorders arising from disruptions in cellular development and associated malformations of cortical development.

Complex instability phenomena in biological and engineered shell structures

Groh, Rainer *(University of Bristol, United Kingdom)* 18:00

The loss of stability or buckling is an important consideration in structural design. More recently, structural instabilities have also been studied in biomechanics, where buckling has been found to be an important mediator of pattern formation. In slender curved shells, commonly found both in lightweight architectures of engineered structures and biological systems, the observed instability phenomena are often complex with a high degree of multistability and featuring interesting dynamics such as pattern formation. A particular challenge is that untangling the governing mechanics that underpin complex instability phenomena often requires more sophisticated computational machinery than is currently available in commercial finite element codes. At a minimum, the elastic nonlinearity that underpins these phenomena requires a means of path-following equilibrium solutions of evolving parameters, broadly classified under the rubric of arc-length solvers. In addition, to fully explore the multi-stable solution landscape, means of automatically detecting possible bifurcations, branching onto alternative paths, or finding remote solutions broken-away from currently known solutions are required. By comprehensively mapping out bifurcation landscapes in this manner, the mechanics governing the onset of buckling, including the role of imperfection sensitivity, can be better understood, and in addition, possibilities for programming adaptive mechanical behaviour can be explored in greater detail. This contribution will outline work conducted by the speaker throughout his five-year Royal Academy of Engineering fellowship in creating suitable computational methods for mapping out complex bifurcation landscapes in shell structures and applying these to uncover pattern formation in engineering and biology. In a traditional engineering context, this presentation will explore the nucleation and subsequent propagation of localised dimples that occur in axially compressed and pressurised cylindrical shells. Depending on the pressurisation of the cylinder, patterns can either form around the cylinder circumference or at an oblique angle. In the biological context, we will explore growth-mediated wrinkling at the edges of plants that lead to the formation of fractal patterns. Here, the role of strongly varying spatial growth fields is especially important in creating residual stresses that lead to buckling and pattern formation. Overall, the ability to

rationalise complex bifurcation spaces with many stable equilibria will be a key prerequisite for engineering programmable structures with tuneable and adaptive behaviour.

YRM3: Emergent behaviour in systems of hydrodynamically interacting particles

Organizer(s): **Höfer, Richard** *(Université de Paris)*
Schubert, Richard *(Universität Bonn)*

YRM3-01: Emergent behaviour in systems of hydrodynamically interacting particles

Date: May 30, 2023 16:30-18:30
Room: CHE/S89

On the (numerical) stability of an equilibria for the Transport Stokes problem

Bonnivard, Matthieu *(Université Paris Cité, France)* 16:30
Mecherbet, Amina *(Université Paris Cité, France)*

The Transport-Stokes system describes sedimentation of a thin suspension of particles in a viscous fluid. It is now well known that the Transport-Stokes system admits a travelling wave solution corresponding to the characteristic function of the unit ball, this result is related to the celerated Hadamard and Rybczynski results which states that a spherical viscous droplet falling in another viscous fluid remains spherical all the time. In this talk, I will first recall well posedness results, the existence of an equilibria for the Transport-Stokes system and a hyperbolic model describing the evolution of the surface of the droplet in the case of axysimmetric initial shapes that can be described through a spherical parametrization. Next I will discuss about some numerical investigations of the stability of the equilibria on both the Transport-Stokes system and the hyperbolic model.

Γ–convergence for nearly incompressible fluids

Bella, Peter *(TU Dortmund, Germany)* 16:50
Feireisl, Eduard *(Czech Academy of Sciences, Czech Republic)*
Oschmann, Florian *(Czech Academy of Sciences, Czech Republic)*

We consider the time-dependent compressible Navier-Stokes equations in the low Mach number regime in a family of domains $\Omega_\epsilon \subset R^d$ converging in the sense of Mosco to a domain $\Omega \subset R^d$, $d \in \{2, 3\}$. We show the limit is the incompressible Navier-Stokes system in Ω, and give some examples of domains Ω_ϵ that fit in our setting. This is joint work with Peter Bella (TU Dortmund) and Eduard Feireisl (CAS).

A connection between homogenisation of compressible Navier-Stokes and fluid-structure problems.

Bravin, Marco *(TU Delft, Netherlands, The)* 17:10

In this talk I will present some recent improvement in the study of homogenization of compressible viscous fluid in the case of tiny holes and the connection with fluid structure problems. In particular I highlight a situation where the fluid + rigid body problem has more flexibility respect to case of the fluid alone. This flexibility helps us to deduce new ideas to study the case of the fluid alone.

Variational approaches to Fluid-Structure Interactions and related problems

Kampschulte, Malte *(Faculty of Mathematics and Physics, Charles University Prague, Czech Republic)* 17:30

In order to rigorously justify macro-scale models, one first needs to deal with the wellposedness of the corresponding model on a micro-scale. For systems of interacting particles, this means studying the problems of fluid-structure interaction. The aim of this talk is to give an introduction to a novel variational technique for proving the existence of global in time weak solutions to large classes of such problems. In particular this technique recently allowed us to extend the time of existence past collisions, which was a problem for large scale limits of independent particles. If time permits, I will also present some preliminary results on a corresponding homogenization problem.

On Implicitly Constituted Fluids with Implicitly Constituted Boundary Conditions

Maringová, Erika *(Institute of Science and Technology Austria)*
Bulicek, Miroslav *(Charles University)*
Malek, Josef *(Charles University)* 17:50

We study systems of nonlinear partial differential equations of parabolic type, in which the elliptic operator is replaced by the first order divergence operator acting on a flux function, which is related to the spatial gradient of the unknown through an additional implicit equation. Formulating four conditions concerning the form of the implicit equation, we first show that these conditions describe a maximal monotone p-coercive graph. We then establish the global-in-time and large-data existence of a (weak) solution and its uniqueness. The theory is tractable from the point of view of numerical approximations. For details, we refer to [1,2].

[1] M. Bulicek, E. Maringova, J. Malek: On nonlinear problems of parabolic type with implicit constitutive equations involving flux, Math. Models Methods Appl. Sci., 31, (2021), no.10, 2039-2090.
[2] M. Bulicek, E. Maringova, J. Malek: On unsteady internal flows of incompressible fluids characterized by implicit constitutive equations in the bulk and on the boundary, (2023), preprint.

Convergence rates for the Stokes-Brinkman equations as homogenisation limit

Jansen, Jonas *(Lunds Universitet, Sweden)* 18:10

Consider $\mathbf{R}^3$ perforated by m moving particles. It is well-known that the Stokes-Brinkman equations appear as homogenisation limit in the critical regime when the particle radius is of order 1/m. In this talk, I will provide an insight on optimal convergence rates and fluctuations for the homogenisation limit. This is joint work with Richard Höfer.

YRM4: Robustness in Deep Learning

Organizer(s): **Croce, Francesco** *(University of Tübingen)*
Thesing, Laura *(LMU München)*

YRM4-01: Robustness in Deep Learning

Date: May 30, 2023 16:30-18:30
Room: HSZ/AUDI

Generalized Hardness of approximation in deep learning – What can we learn with neural networks?

Thesing, Laura *(LMU Munich, Germany)* 16:30
Bastounis, Alexander *(University of Edinburgh)*
Hansen, Anders Christian *(University of Cambridge)*

The impact deep learning and artificial intelligence have on our daily lives, and society can hardly be overestimated. The use cases vary from health care to migration and law decisions. Especially in these highly sensitive areas, the robustness of the methods is of utmost importance. The European Commission now also requires robustness, security and accuracy for all tasks where the decision of the system has a direct impact on people's life. However, besides the tremendous success of state-of-the-art deep learning methods, there is a large variety of empirical evidence showing robustness issues like hallucinations and adversarial examples. These experiments have recently been underlined by publications showing the limitations of deep learning on digital machines, i.e., the computers we are currently using. Especially, it has been shown that there are problems, for example, inverse problems, for which neural networks exist for the solution but no algorithm can compute them. This shows clear theoretical limitations of neural networks and deep learning beyond the empirical evidence of the robustness issues. n sensitive applications we need to be able to give guarantees on the accuracy of the algorithm. However, infinite accuracy is rarely necessary. Therefore, we want to consider the generalized hardness of approximation for deep learning with neural networks. The concept is a generalization of the hardness of approximation, which given P $\neq$NP, says that for $\epsilon > \epsilon_0$ solutions can be computed but for $\epsilon < \epsilon_0$ the solution becomes intractable. In a similar spirit, we study the approximation of functions with neural networks. Then we investigate the boundary ϵ_0 for approximating functions by an algorithm and ϵ_1 for the approximation with neural networks. Given the limitations, in terms of the computability of neural networks in deep learning, we aim to give insight into what is possible with neural networks and extend the given approximation theoretical results to realizability in practice.

How to quickly obtain models robust to multiple threats, and their advantages

Croce, Francesco *(University of Tübingen, Germany)* 16:50

Several methods have been proposed to train classifiers robust to a single adversarial attack. However, such models are still vulnerable to perturbations different from those seen at training time: For example, training with l_∞-bounded attacks does not yield good robustness in

the l_1-threat model. Moreover, the existing methods for simultaneous robustness to multiple attacks need to use all of them at training time, and are computationally expensive. First, we show that a short fine-tuning can turn a classifier initially robust to l_p-bounded perturbations into one robust to another threat model, e.g., l_q for $p \neq q$. Second, taking advantage of the geometry of l_p-balls, we suggest that training with l_∞- and l_1-attacks is sufficient to obtain robustness to the intermediate l_p-attacks. Then, combining these two elements, we can obtain classifiers with multiple norm robustness at small computational cost. Finally, we show that such models might have desirable properties, like being more robust to unseen, non-l_p-bounded attacks, and better explainability.

Still no free lunch – On hallucinations and non-robustness in AI for imaging

Antun, Vegard *(University of Oslo, Norway)* 17:10

Methods inspired by AI are currently entering medical imaging with full force. Yet, there is also increasing empirical evidence showing that these new methods are susceptible to AI generated hallucinations, the phenomenon where realistically looking artefacts are incorrectly added to the reconstructed image, causing serious concerns in the sciences. The basic question is therefore: can hallucinations be prevented? In this talk, we present a comprehensive mathematical analysis explaining the many facets of AI generated hallucinations in imaging, their links to instabilities, but also how stable AI methods can hallucinate. Several of our results take the form of "no free lunch" theorems and are valid for arbitrary reconstruction methods, not just for AI-inspired techniques. Specifically, we will show that (i) methods that overperform on a single image can wrongly transfer details from one image to another, creating a hallucination, (ii) hallucinations can occur for any probability distribution on the data used, yet non-hallucinating algorithms exist, (iii) reconstruction methods with over- or inconsistent performance can produce both hallucinations and instabilities, and it is generally difficult to mitigate these effects, (iv) it may be impossible to construct optimal reconstruction maps for certain problems. Our results trace these effects to the kernel of the forward operator and assert that hallucinations and instabilities can be avoided only if information about the kernel is encoded into the reconstruction procedure.

Towards Reliable Graph Neural Networks

Zügner, Daniel *(Microsoft Research, Germany)* 17:30

This talk discusses the reliability of GNNs, specifically their robustness with respect to adversarial attacks, and their ability to estimate predictive uncertainty. We show how to obtain robustness certificates for perturbations of the node attributes as well as changes to the graph structure, and how to train up to 4x more robust GNNs.

Understanding robustness in the parameter space of deep networks

Andriushchenko, Maksym *(EPFL, Switzerland)* 17:50

Part 1. Sharpness-Aware Minimization (SAM) is a recent training method that relies on worst-case weight perturbations which significantly improves generalization in various settings. We argue that the existing justifications for the success of SAM which are based on a PAC-Bayes generalization bound and the idea of convergence to flat minima are incomplete. Moreover,

there are no explanations for the success of using m-sharpness in SAM which has been shown as essential for generalization. To better understand this aspect of SAM, we theoretically analyze its implicit bias for diagonal linear networks. We prove that SAM always chooses a solution that enjoys better generalization properties than standard gradient descent for a certain class of problems, and this effect is amplified by using m-sharpness. We further study the properties of the implicit bias on non-linear networks empirically, where we show that fine-tuning a standard model with SAM can lead to significant generalization improvements. Finally, we provide convergence results of SAM for non-convex objectives when used with stochastic gradients. We illustrate these results empirically for deep networks and discuss their relation to the generalization behavior of SAM.

Part 2. Sharpness of minima is a promising quantity that can correlate with generalization in deep networks and, when optimized during training, can improve generalization. However, standard sharpness is not invariant under reparametrizations of neural networks, and, to fix this, reparametrization-invariant sharpness definitions have been proposed, most prominently adaptive sharpness (Kwon et al., 2021). But does it really capture generalization in modern practical settings? We comprehensively explore this question in a detailed study of various definitions of adaptive sharpness in settings ranging from training from scratch on ImageNet and CIFAR-10 to fine-tuning CLIP on ImageNet and BERT on MNLI. We focus mostly on transformers for which little is known in terms of sharpness despite their widespread usage. Overall, we observe that sharpness does not correlate well with generalization but rather with some training parameters like the learning rate that can be positively or negatively correlated with generalization depending on the setup. Interestingly, in multiple cases, we observe a consistent negative correlation of sharpness with OOD generalization implying that sharper minima can generalize better. Finally, we illustrate on a simple model that the right sharpness measure is highly data-dependent, and that we do not understand well this aspect for realistic data distributions.

Training machine learning models with malicious teachers

Cinà, Antonio Emanuele *(CISPA Helmholtz Center for Information Security, Germany)* 18:10

The recent success of machine learning (ML) has been fueled by the increasing availability of computing power and large amounts of data in many different applications. However, the trustworthiness of the resulting models can be compromised when such data is maliciously manipulated to mislead the learning process. In this talk, we first review poisoning attacks that compromise the training data used to learn ML models, including attacks that aim to reduce the overall performance, manipulate the predictions on specific test samples, and even implant backdoors in the model. We then discuss how to mitigate these attacks using basic security principles or deploying ML-oriented defensive mechanisms. We conclude the discussion by formulating some relevant open challenges hindering the development of testing methods and benchmarks suitable for assessing and improving the trustworthiness of ML models against data poisoning attacks.

YRM5: Material Modelling Across Length Scales

Organizer(s): **Waimann, Johanna** *(RWTH Aachen)*
Kaiser, Tobias *(TU Dortmund)*

YRM5-01: Material Modelling Across Length Scales

Date: May 30, 2023 16:30-18:30
Room: POT/51

Efficient thermo-mechanically coupled FE-FFT-based multiscale simulation of polycrystals

Gierden, Christian *(RWTH Aachen University, Germany)* 16:30
Schmidt, Annika *(RWTH Aachen University, Germany)*
Waimann, Johanna *(RWTH Aachen University, Germany)*
Svendsen, Bob *(RWTH Aachen University, Germany; Max-Planck-Institut für Eisenforschung GmbH, Germany)*
Reese, Stefanie *(RWTH Aachen University, Germany)*

In general, the overall material behavior of any structural component is directly dependent on its underlying microstructure, which for metal components is given in terms of a polycrystal. To enable the simulation of the associated microstructural and overall material behavior, a two-scale simulation approach can be applied. In this context, we use the FE-FFT-based two-scale method [1], which is an efficient alternative to the classical FE^2 approach for the simulation of periodic microstructures [2]. Using the FE-FFT-based two-scale method, the finite element (FE) method is applied to solve the macroscopic boundary value problem and the fast Fourier transform (FFT)-based simulation technique is used to deal with the microscopic boundary value problem. In addition, we consider a thermo-mechanically coupled framework to account for both thermal and mechanical loads and implement an elasto-viscoplastic material model. Finally, we incorporate a model order reduction technique based on a coarsely discretized microstructure [3, 4] to develop an efficient two-scale simulation scheme. Several numerical examples are used to demonstrate the feasibility of the proposed simulation framework.

[1] Spahn, J., Andrä, H., Kabel, M., & Müller, R. (2014). A multiscale approach for modeling progressive damage of composite materials using fast Fourier transforms. Computer Methods in Applied Mechanics and Engineering, 268, 871-883.
[2] Gierden, C., Kochmann, J., Waimann, J., Svendsen, B., & Reese, S. (2022). A review of FE-FFT-based two-scale methods for computational modeling of microstructure evolution and macroscopic material behavior. Archives of Computational Methods in Engineering, 29(6), 4115-4135.
[3] Kochmann, J., Wulfinghoff, S., Ehle, L., Mayer, J., Svendsen, B., & Reese, S. (2018). Efficient and accurate two-scale FE-FFT-based prediction of the effective material behavior of elasto-viscoplastic polycrystals. Computational Mechanics, 61, 751-764.
[4] Gierden, C., Kochmann, J., Waimann, J., Kinner-Becker, T., Sölter, J., Svendsen, B., & Reese, S. (2021). Efficient two-scale FE-FFT-based mechanical process simulation of elasto-viscoplastic polycrystals at finite strains. Computer Methods in Applied Mechanics and Engineering,

374, 113566.

Modeling intragranular slip localization modes within polycrystals

Marano, Aldo *(Onera, Université Paris-Saclay, Materials and Structures Department, 29 av. Division Leclerc, 92320 Châtillon, France)*
Forest, Samuel *(MINES ParisTech, PSL University, Centre des matériaux, CNRS UMR 7633, Evry, Franc)*
Gélébart, Lionel *(Université Paris-Saclay, CEA, Service de Recherches Métallurgiques Appliquées, Gif-sur-Yvette, France)*

16:50

Intragranular localization of plastic slip plays a key role in the deformation and fracture mechanisms of polycrystalline materials. As shown by Asaro & Rice [1], softening crystal plasticity (CP) equations predict the formation of two types of localization bands as bifurcation modes in homogeneous crystals: slip bands and kink bands. With the advances of high performance numerical simulation, those equations can be integrated over large polycristalline unit cells with a high-resolution, in order to bridge together the localization band and polycrystalline scales. This work explores the potential of this approach to achieve accurate simulation of slip localization and its consequences on polycrystalline materials mechanics, through massively parallel FFT-based simulations [2].

First, the ability of the classical crystal plasticity theory to simulate intense slip localization bands will be presented, supported by a systematic analysis of full field simulations to characterize localization bands geometry, number and nature. It is shown that classical CP models fundamentally cannot accurately predict realistic bands networks, as they predict slip and kink bands as two equivalent localization modes. Hence, they predict similar amounts and characteristics for both type of bands, whereas in reality they are two distinct phenomena.

To break the modes equivalence, the benefits of using a class of Nye's tensor based gradient plasticity models [3] will be exposed. It is evidenced that these models change qualitatively the nature of simulated slip localization. They significantly reduce the amount of simulated kink bands, allow to control their width through the model characteristic length and predict their formation as a dense succession of slip bands, in accordance with observation. Hence, this modeling approach yields more sound localization band networks in polycrystalline simulation results.

Finally, ongoing work exploring the inclusion of more characteristic lengths related to plasticity localization bands to progress towards a quantitative simulation of localization band networks will be discussed.

[1] Asaro, R., Rice, J., 1977. *Strain localization in ductile single crystals*. J. Mech. Phys. Solids 25, 309-338
[2] Schneider, M. *A review of nonlinear FFT-based computational homogenization methods*. *Acta Mech* (2021)
[3] Gurtin, M.E., 2002. *A gradient theory of single-crystal viscoplasticity that accounts for geometrically necessary dislocations.* J. Mech. Phys. Solids 50, 5-32.

Multiscale and Multiphase Simulation of Function-Perfusion Processes in the Liver on Whole Body, Organ, Lobule, and Cell Scale

Lambers, Lena *(Institute of Structural Mechanics and Dynamics, Faculty for Aerospace Engineering and Geodesy, University of Stuttgart, Germany; Experimental Transplantation Surgery, Department of General, Visceral and Vascular Surgery, Jena University Hospital, Germany)*
Gerhäusser, Steffen *(Institute of Structural Mechanics and Dynamics, Faculty for Aerospace Engineering and Geodesy, University of Stuttgart, Germany)*
Mandl, Luis *(Institute of Structural Mechanics and Dynamics, Faculty for Aerospace Engineering and Geodesy, University of Stuttgart, Germany)*
Ricken, Tim *(Institute of Structural Mechanics and Dynamics, Faculty for Aerospace Engineering and Geodesy, University of Stuttgart, Germany)*

17:10

As a central organ for vital metabolic processes, the liver has a complex interplay of perfusion and functional processes on different length scales. On the organ scale, macroscopic perfusion processes in a branching vascular tree determine the input for the microcirculation through the capillaries coupled to function processes in liver cells. To better understand the interplay between hepatic perfusion, metabolism and tissue in the hierarchically organized liver structure, we have developed a multicomponent, poroelastic multiphase and multiscale function-perfusion model, cf. [1], using a multicomponent mixture theory based on the Theory of Porous Media (TPM, see [2]). The computation of the branching vascular tree on the organ scale enables the calculation of macroscopic pressure and velocity changes, for example, after surgical interventions for tumor removal. On the lobular scale, we assume a homogenized tetra-phasic mixture body, composed of a porous solid structure representing healthy tissue, a liquid phase describing the blood, and two solid phases with the ability of growth and depletion representing fat and tumor tissue as well as solutes solved in the phases. On the cellular scale, systems biology models are implemented to describe the metabolism as well as the production, utilization and storage of the metabolites in the cells. To further incorporate metabolic processes in the body, a whole-body model provides metabolic changes from kidney or lung during the circulation of the blood through the body. The describing PDEs on the lobular scale are coupled with ODEs on the cell and whole-body scale using a coupling library resulting in a tri-scale PDE-ODE approach. A special focus here is on the boundary conditions that represent the blood flow through the liver lobules. To increase the robustness of the model and allow for near real-time patient-specific simulations, computationally critical parts of the model are enhanced by data-driven methods through the integration of experimental, clinical and in silico data from cooperation partners [3,4].

[1] Ricken, T., et al. BMMB (2015) 14:515-536
[2] Ehlers, W. Foundations of multiphasic and porous materials (2002)
[3] Christ, B., [...], Lambers, L., [...], Ricken, T., et al. Frontiers in Physiology (2021) 12
[4] Seyedpour, S.M., [...], Lambers, L. [...] and Ricken, T. Frontiers in Physiology (2021) 12

Numerical model reduction in computational homogenization of fractured porous media

Ekre, Fredrik *(Institute of Applied Mechanics, TU Braunschweig, Germany)*
Gräßle, Carmen *(Institute for Partial Differential Equations, TU Braunschweig, Germany)*
Jänicke, Ralf *(Institute of Applied Mechanics, TU Braunschweig, Germany)*

17:30

Computational homogenization can be used in order to model the effective mechanical behavior of fluid saturated porous rock with heterogeneous properties. A standard approach is the "finite element squared" (FE^2) procedure, where a new boundary value problem for the coupled porous media problem is defined on a Representative Volume Element (RVE). The effective macroscopic response is obtained from solving the RVE problem. The FE^2 strategy can be computationally expensive and it is therefore of interest to reduce the cost of solving the individual RVE problems by introducing a reduced basis.

A well known method for identifying a reduced basis is Proper Orthogonal Decomposition (POD), which has also been used in the context of homogenization of porous media[1]. Typically POD basis reduction can be split into an "offline" stage and an "online" stage. During the offline stage a set of training computations are performed in order to collect snapshots of the system. These snapshots are then used to construct a POD basis. In the online stage the simulation is accelerated by using the reduced basis. Naturally the accuracy of the online simulation depends on how well the reduced basis can capture also the new conditions.

This definitive split between an offline and online stage is not always a good strategy since it is not always feasible to exhaustively train the model to account for every possible "online scenario". One application where this is particularly difficult is crack propagation since i) it is difficult to construct suitable training conditions that capture all the possible crack paths that might happen in the online phase and ii) a growing crack may suddenly and drastically change the dynamics of the problem since the permeability of an open crack is much higher than the surrounding matrix material. Given these difficulties it would be desirable to detect when the (original) basis become inaccurate, and then adapt the basis, during the online phase, for the new conditions.

In this presentation we enhance the model presented in [2] with a phase-field description of cracks to investigate the effect on the homogenized properties. We also present preliminary results for an adaptive basis that can adjust for the new physics as the crack grows.

Reaching larger length and time scales in atomistic simulations via statistically averaged coarse graining

Saxena, Shashank *(ETH Zurich, Switzerland)*
Spinola, Miguel *(ETH Zurich, Switzerland)*
Gupta, Prateek *(IIT Delhi, India)*
Kochmann, Dennis M. *(ETH Zurich, Switzerland)*

17:50

Atomistic simulations using conventional molecular dynamics are limited in length and time scales due to the short time steps of explicit integration schemes and a significant increase in the number of degrees of freedom in a large simulation domain. Finite-temperature MD simulations therefore usually employ the use of periodic boundary conditions with small domain sizes and unrealistically high loading rates. However, natural heat and mass transport

processes occur at different length and time scales and are hence inaccessible by MD simulations. Simulating such long-term processes requires tracking the statistically averaged phase space coordinates of the system rather than resolving dynamics in the fine-grained phase space. The Gaussian Phase Packets (GPP) approach is one such formulation, which posits a Gaussian distribution of atomic positions and momenta, and finds the parameters of the distribution which minimize the free energy of the system. Upscaling in length is achieved by using the quasicontinuum (QC) framework which performs a spatial coarse-graining of the atomic ensemble by solving for the positions of some chosen representative atoms and interpolating between them to obtain the position of others. Coupled with techniques to explore the free energy landscape, such as the nudged elastic band (NEB) and the dimer method, the GPP formulation can be used to investigate transformation mechanisms and simulate the diffusion of substitutional and interstitial impurities in the solvent at longer time scales.

We first discuss the GPP formulation in the quasistatic limit where it involves iteratively solving a set of coupled nonlinear equations to satisfy vanishing phase-averaged physical and thermal forces at each atomic site. The phase averaging of forces and potential energy is performed by integrating over the entire phase space. Applications to study finite-temperature surface elastic parameters and symmetric-tilt grain boundary energies are discussed. Followed by this, we study minimum energy pathways (MEP) for the martensitic phase transition in iron using the NEB on a GPP-based free energy landscape and vacancy migration and void growth at finite temperatures in pure metals. We discuss the advantages and limitations of this framework to study mass transport in crystals and demonstrate its computational efficiency to overcome the length and time-scale limitations of MD.

Second-order computational homogenization of fluid flow in porous media

Polukhov, Elten *(University of Stuttgart, Germany)*
Khurshid, Hamza *(University of Stuttgart, Germany)*
Keip, Marc-André *(University of Stuttgart, Germany)*

18:10

In the present contribution, we develop a second-order computational homogenization framework for fluid-saturated porous media at small strains. The model will be based on a minimization-type variational formulation that extends the first-order computational-homogenization framework documented in [2]; see also [1]. As a result, we treat the fluid-transport problem in a heterogeneous porous medium across two scales that are not strictly separated. While the macroscopic response will be governed by a second-gradient approach [3,5], the microscopic problem will be based on a Cauchy continuum and Biot's first-gradient theory. Nonetheless, the microscopic displacement and fluid-flux fields are enriched with the first- and second-order contributions from the macroscopic scale. Next to the theoretical framework, we will also discuss a suitable space-time discretization alongside some numerical examples that are aimed to showcase the overall model response.

References

[1] C. Miehe, S. Mauthe and S. Teichtmeister. Minimization principles for the coupled problem of Darcy-Biot-type fluid transport in porous media linked to phase field modeling of fracture. Journal of the Mechanics and Physics of Solids, 82, 186-217 (2015).

[2] E. Polukhov and M.-A. Keip. Computational homogenization of transient chemo-mechanical processes based on a variational minimization principle. Advanced Modeling and Simulation in Engineering Sciences, 7, 1-26 (2020).
[3] I. A. Rodrigues Lopez, and F. M. Andrade Pires. Unlocking the potential of second-order computational homogenisation: An overview of distinct formulations and a guide for their implementation. *Archives of Computational Methods in Engineering*, 1-55 (2021).
[4] G. Sciarra, F. dell'Isola, and O. Coussy. Second gradient poromechancis. International Journal of Solids and Structures, 44, 6607-6629 (2007).
[5] J. Yvonnet, N. Auffray and V. Monchiet. Computational second-order homogenization of materials with effective anisotropic strain-gradient behavior. International Journal of Solids and Structures, 191-192, 434-448 (2020).

YRM6: Parameter Identification

Organizer(s): **Jurgelucks, Benjamin** *(HU Berlin)*
Schäfer, Kai *(Universität Bremen)*

YRM6-01: Parameter Identification

Date: May 30, 2023 16:30-18:30
Room: HSZ/H02

Benchmarking Methods for Parameter Identification in Dynamical Systems

Wiesner, Marek *(University of Bremen, Germany)* 16:30
Büskens, Christof *(University of Bremen, Germany)*

Accurate models are essential for simulating, optimizing, and controlling real-world processes. Such processes are often modeled with a parameter-dependent ordinary differential equation (ODE). The task of identifying the parameters with the help of measurements of a specific process is challenging and can be approached in different ways. Many approaches to identify the model parameters minimize the distance between the model output and the measurements. To obtain the model output, these classical techniques approximate the solution of the ODE numerically. Shooting methods, where the ODE is solved by an external integration scheme, are among the classical approaches. Another method in this class is full discretization. Here, new variables are introduced that describe the discretized model output. An integration scheme is then formulated as a constraint to ensure that the new variables approximate a solution of the ODE. Since the solution of the ODE can be sensitive to initial values and model parameters, finding a global minimum of the resulting optimization problem is challenging. Additionally, the approaches can be computationally expensive, making them potentially impracticable for large-scale problems. The class of gradient matching methods approaches parameter identification differently. Classically, these methods consist of two steps. The first step is to approximate the slope of the measurements. A simple way of doing this is computing a spline approximation of the measurements and taking its derivative as the measurement slope. In the second step, the model parameters are identified by minimizing the distance between the measurement slope and the state derivatives obtained from the ODE. Thus, gradient matching methods avoid solving the ODE. The main challenge is to find a suitable approximation of the measurement slope, as the parameter identification depends heavily on its quality. As discussed in the previous sections, there is a wide variety of parameter identification methods, each with advantages and disadvantages. In general, it is unclear which method works well for a particular problem. This talk presents a benchmark of different methods for parameter identification from both classical and gradient matching approaches. Their performance is analyzed and systematically compared on a database of test problems. It is investigated if there is a notable difference in the performance of the various methods and if one approach is superior to the others. Ultimately, these results can be used in the decision-making of choosing a method for a particular parameter identification problem.

Symmetry detection combined with Hamiltonian neural networks

Dierkes, Eva *(University of Bremen, Germany)*
Offen, Christian *(Paderborn University, Germany)*
Ober-Blöbaum, Sina *(Paderborn University, Germany)*
Flaßkamp, Kathrin *(Saarland University, Germany)*

17:00

Machine learning methods rapidly develop in various applications, such as computer vision or gameplay. Data-based methods such as deep neural networks possess high flexibility in approximating functions. As these methods are used for various applications, they have also come to be used to model dynamical systems. Furthermore, if the system is known to be Hamiltonian, particular neural network architectures like 'Hamiltonian Neural Networks' (HNN) can be used as they learn the underlying structure. Even though HNNs are designed to preserve the symplectic structure, they often fail to obey other physical laws.
Mechanical systems often come with other system structures, such as system symmetries. The conventional HNN neglects modelling these additional structures. If the considered mechanic system possesses symmetries, it significantly improves the model if they are preserved during the data-driven modeling.
In this work, we propose to augment Hamiltonian Neural Networks with a Lie Algebra framework to detect systems symmetries alongside learning the Hamiltonian. The detected symmetry is additionally embedded in Hamiltonian learning. The proposed framework is able to discover and embed affine linear transformations, as shown on the pendulum on a cart and on the two-body example. The prediction with our learned 'Symmetry HNN' (SymHNN) outperforms HNNs without symmetry learning.

Identification of the basal drag parameter in ice sheet models

Höyns, Lea-Sophie *(Alfred-Wegener-Institut, Helmholtz-Zentrum für Polar- und Meeresforschung, Bremerhaven, Germany; University of Bremen, Center for Industrial Mathematics, Bremen, Germany)*
Kleiner, Thomas *(Alfred-Wegener-Institut, Helmholtz-Zentrum für Polar- und Meeresforschung, Bremerhaven, Germany)*
Rademacher, Andreas *(University of Bremen, Center for Industrial Mathematics, Bremen, Germany)*
Rückamp, Martin *(Bavarian Academy of Sciences and Humanities, München, Germany)*
Wolovick, Michael *(Alfred-Wegener-Institut, Helmholtz-Zentrum für Polar- und Meeresforschung, Bremerhaven, Germany)*
Humbert, Angelika *(Alfred-Wegener-Institut, Helmholtz-Zentrum für Polar- und Meeresforschung, Bremerhaven, Germany; University of Bremen, Department of Geosciences, Bremen, Germany)*

17:30

In the application of glaciology, parameter identification problems occur due to the fact that some relevant parameters are difficult to observe directly, like the distribution of the basal drag underneath the ice sheets. However, it has a strong influence on sliding and thus an impact on ice flow speeds. With that, it is also important for making realistic projections of

future ice sheet behavior. This results in the urgent need to determine the associated basal drag parameter in the ice sheet models.

These parameter identification problems can be solved by the help of gradient based optimization algorithms using adjoint equations. Which is an effective way to infer model parameters, like the basal drag parameter, in a way that the misfit between modeled and observed surface velocity is minimized. The model equations are represented through a Full-Stokes approximation of the momentum balance, and the unknown parameter to be controlled is contained in the boundary conditions at the ice base interface. A regularization term is added to the costfunction to improve the numerical stability by penalizing oscillations in the gradient of the basal drag parameter. This additional term is equipped with a weight which can be derived by performing an L-curve analysis.

Here, we conduct the parameter identification within the finite-element based Ice-sheet and Sea-level System Model (ISSM) in order to determine the basal drag parameter for the West Antarctic Ice Sheet. We employ a non-linear Budd friction law acting beneath the ice sheet. To achieve more realistic results, we include into this friction law the effective pressure simulated using a subglacial hydrological model, the confined-unconfined aquifer system model CUAS-MPI.

We present our approach behind the parameter identification in ice sheet models. We show the distribution of the determined basal drag parameter, discuss its spatial variability as well as further results of the model procedure like the basal drag.

Inverse procedure for the identification of piezoelectric material parameters supported by dense neural networks

Claes, Leander *(Paderborn University, Germany)*
Meihost, Lars *(Paderborn University, Germany)*
Jurgelucks, Benjamin *(Humboldt-Universität zu Berlin, Germany)*

18:00

The accurate knowledge of quantitative material parameters is a prerequisite for simulation-driven design processes of piezoelectric sensors and actuators. Due to the large number of parameters required to describe the mechanical, electrical, and coupling behaviour of theses materials, the identification procedure is especially challenging. In this contribution we aim to identify a full set of piezoelectric material parameters using a single disc-shaped sample. This is achieved by implementing an inverse measurement procedure based on matching the measured impedance of the physical sample with the output of a finite-element simulation model, the forward model. Because gradient-based, local optimisation is used for the identification process, an initial estimate for the parameters is required. For this initial value estimation, the forward model is inverted using a dense neural network. Synthetic training data for the neural network is generated by evaluating the forward model an adequate number of times with randomised material parameters. The network architecture is chosen so all directly measurable quantitate, i.e. the samples of the impedance in frequency domain as well as the density are the input of the network, while the material parameters are the output of the network. After training is concluded, the measured quantities are supplied to the neural network, which yields the initial estimates for the material parameters. A forward

simulation using these results shows good agreement with the physical behaviour of the sample, enabling an efficient gradient based optimisation in the subsequent, final step of material parameter identification.

DFG Priority Programs

PP 1886: Polymorphic Uncertainty Modelling for the Numerical Design of Structures

Organizer(s): **Kaliske, Michael** *(TU Dresden)*

PP 1886-01: Polymorphic Uncertainty Modelling for the Numerical Design of Structures

Date: May 30, 2023 13:30-16:10
Room: HSZ/204

Artificial neural network surrogate modeling for uncertainty quantification and structural optimization of reinforced concrete structures

Freitag, Steffen *(Karlsruhe Institute of Technology, Germany)* 13:30
Edler, Philipp *(Ruhr University Bochum, Germany)*
Schoen, Stefanie *(Ruhr University Bochum, Germany)*
Meschke, Günther *(Ruhr University Bochum, Germany)*

Optimization approaches are important to design sustainable structures. In structural mechanics, different design objectives can be defined, e.g., to minimize the required construction material or to maximize the structural durability. In addition to the objectives of an optimization problem, constraints with respect to the structural safety and serviceability have to be considered, e.g., stress and displacement constraints. The structural behavior with respect to the applied loads needs to be described by adequate numerical models to evaluate the quantities of interest representing the design objectives and constraints. For the durability assessment of reinforced and fiber reinforced concrete structures, advanced finite element (FE) models are used to simulate the cracking behavior. The maximal crack width is often used as an indicator for the structural durability. If also the chloride transport process of the cracked reinforced concrete structure is simulated, it is possible to consider the corrosion initiation as an additional durability measure. The variability of structural loads and material parameters and unavoidable construction imprecisions leads to a probabilistic reliability and durability assessment, where aleatory as well as epistemic uncertainties are quantified by random variables, intervals and probability-boxes. However, FE simulation models cannot directly be applied to structural analyses and optimizations with polymorphic uncertain parameters and design variables because of the high computational demand of the multi-loop algorithms (Monte Carlo simulation, interval analysis, global optimization). In this presentation, artificial neural network surrogate modeling approaches are shown, to speed-up the uncertainty quantification and structural optimization of reinforced concrete structures.

Incorporating Uncertainty in Stress-Strain Data Acquisition: Extended Model-Free Data-Driven Identification

Zschocke, Selina *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*
Graf, Wolfgang *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*
Kaliske, Michael *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*

13:50

Based on the increasing ability to collect and store large amounts of data, data-driven methods have recently gained importance in the context of computational mechanics. Compared to the traditional approach of defining a suitable constitutive model and fit the parameters to experimental data, these methods aim to capture complex material behaviour without the assumption of a certain material model. Distinguished are model-based data-driven methods, leading to an approximation of the constitutive material description e.g. by neural networks, and model-free data-driven methods. The approach of data-driven computational mechanics (DDCM), introduced by Kirchdoerfer and Ortiz (2016), enables to circumvent any material modelling step by directly incorporating material data into the structural analysis. A basic prerequisite for both types of data-driven methods is a large amount of data representing the material behaviour, in solid mechanics consisting of stresses and strains. Obtaining these databases numerically by multiscale approaches is computationally expensive and requires the definition of lower scale models. In case of an experimental characterization, constitutive descriptions are generally required to compute the stress states corresponding to displacement fields, e.g. identified by full-field measurement techniques, such as digital image correlation.

The method of data-driven identification (DDI), introduced in Leygue et al. (2018) based on the principles of DDCM, enables the determination of detailed information about the constitutive behaviour based on displacement fields and applied boundary conditions without a specific material model. Stresses corresponding to given strains are identified by iteratively clustering and enforcing equilibrium. The algorithm has shown to be applicable to synthetic as well as real data taking linear and non-linear material behaviour into account. In order to obtain realistic simulation results, uncertainty needs to considered. Generalized polymorphic uncertainty models, resulting as a combination of aleatoric and epistemic uncertainty models, are utilized to take variability, imprecision, inaccuracy and incompleteness of data into account. The consideration of uncertain material properties by data-driven simulation approaches leads to the requirement of data sets representing uncertain material behaviour. In this contribution, different sources of uncertainty occurring within data-driven identification of stress-strain relations are addressed and an efficient method for the identification of data sets representing uncertain material behaviour based on the concept of DDI is proposed. In order to demonstrate the developed methods, numerical examples are carried out.

Reduced order modeling of structural problems with damage and plasticity

Kehls, Jannick *(Institute of Applied Mechanics, RWTH Aachen University, Germany)*
Kastian, Steffen *(Institute of Applied Mechanics, RWTH Aachen University, Germany)*
Brepols, Tim *(Institute of Applied Mechanics, RWTH Aachen University, Germany)*
Reese, Stefanie *(Institute of Applied Mechanics, RWTH Aachen University, Germany)*
14:10

The study of structural problems in engineering fields is crucial in ensuring the safety and longevity of structures. In particular, the consideration of damage and plasticity in these structures is important as it can affect the performance and overall integrity of the structure. Model order reduction techniques (MOR) are used to reduce the computational effort of the damage and plasticity simulations.

MOR methods reduce the simulation effort by representing the problem using a lower number of degrees of freedom. The use of reduced order models (ROM) in the analysis of structural problems with damage and plasticity has the potential to significantly reduce computational time and increase efficiency. Of course, the approximation of a problem in a lower dimensional space introduces an approximation error, that needs to be kept small enough so that the results of the MOR maintain their validity.

One well-known reduced-order modeling approach is the proper orthogonal decomposition (POD). POD is used to extract the dominant modes of the structure, which are then used to solve a problem in the smaller dimensional subspace. To overcome the limitations of POD regarding nonlinear problems, the discrete empirical interpolation method (DEIM) [1] is employed. The successful application of the DEIM to nonlinear structural mechanics with hyperelastic and viscoelastic material behavior has for example been shown in [2].

Because material models concerned with damage exhibit phenomena such as softening and snap-back [3], the arc-length method needs to be employed to solve the problem efficiently. Concerning the ROM, a reduced arc-length method is proposed. Whether the reduced form of the arc-length method still leads to stable simulations is still under research. It is also investigated whether the approximation accuracy of the combination of the aforementioned methods is high enough for real engineering applications.

[1] S. Chaturantabut and D. C. Sorensen, SIAM J. Sci. Comput. 32(5): 2737-2764, 2010
[2] A. Radermacher and S. Reese, Int. J. Numer. Methods Eng. 107(6): 477-495, 2016
[3] T. Brepols, S. Wulfinghoff, and S. Reese, Int. J. Plast. 129, 102635, 2020

Incorporation of the IGA-FEM basis functions into the non-deterministic FEM-framework

Pivovarov, Dmytro *(FAU Erlangen-Nürnberg, Germany)*
Steinmann, Paul *(FAU Erlangen-Nürnberg, Germany)*
Willner, Kai *(FAU Erlangen-Nürnberg, Germany)*
14:30

The objective of this study is to generalize the advanced IGA-FEM for the general non-deterministic (fuzzy-interval-stochastic) problem setting. We use the IGA-FEM basis functions to model the dependence of the solution field on uncertain parameters in the parametric domain as well as in the physical domain, where IGA-FEM traditionally is used to approximate the solution of the partial differential equation. Our approach to handling uncertainties is based on a low-rank tensor representation of the solution field and an adaptive sampling.

The corresponding algorithms are shown, along with some application examples. The advanced IGA-FEM approximation of the solution field in the parametric domain, which exhibits high smoothness and oscillation-free behavior, is a crucial part of the effective sampling algorithm.

Polymorphic Uncertainty Quantification for the Additive Manufacturing of Elastic Rods

Wolff-Vorbeck, Steve *(University of Freiburg, Germany)*
Luo, Yongming *(Technische Universität Dresden, Germany)*
Dondl, Patrick *(University of Freiburg, Germany)*
Neukamm, Stefan *(Technische Universität Dresden, Germany)*
Schulz, Alexander *(University of Freiburg, Germany)*

14:50

For some time now, additive manufacturing has been a widespread method in a huge variety of engineering applications. Overall, its nearly limitless design freedom has enabled the practice of trial and error approaches in many fields of bio- and civil-engineering. However, one needs to consider different errors introduced on the designs due to the manufacturing process and especially, evaluate the effect of these errors on the mechanical properties of the structure. Indeed, the variability in certain mechanical properties of manufactured objects might be significant and thus the application of uncertainty quantification techniques is crucial in the pre-production process.

We, therefore, derive comprehensive models enabling an efficient uncertainty quantification of mechanical properties for additively manufactured rod-shaped elastic solids in terms of errors introduced within the manufacturing process.

Here, we consider the fused-filament-fabrication process where the main sources of uncertainties are given by geometric deviations of the printed object from the designed object and by variations of material properties caused by fluctuation of material density. The 3d-printed objects investigated in this work are made of polycarprolactone, a bioresorbable, biocompatible, polymer-based material, which is commonly used in the engineering of patient specific bone scaffolds. We then deduce a comprehensive modelling approach in three space dimensions for determining different effective mechanical properties of randomly perturbed elastic rods where we consider both aleatoric and epistemic uncertainties in the representation of the perturbations.

To do so, we use the polymorphic uncertainty model of fuzzy structural analysis including the representation of random perturbations as fuzzy random fields and perform an alpha-level optimization using Monte-Carlo simulations combined with finite element methods.

Furthermore, we introduce an one-dimensional surrogate model for rod-shaped elastic solids with fixed cross-section. By this the problem can be reduced to an one-dimensional optimization problem requiring only the solution of a system of ordinary differential equations. This leads to a marked reduction of computational effort compared to the three-dimensional model concerning the computation of mechanical properties of randomly perturbed elastic rods.

Preconditioner for iterative solvers for numerical models under polymorphic uncertainty

Schmidt, Albrecht *(Materials Research and Testing Institute at the Bauhaus-Universität Weimar, Germany)* 15:10

Lahmer, Tom *(Materials Research and Testing Institute at the Bauhaus-Universität Weimar, Germany; Bauhaus-Universität Weimar, Germany)*

Iterative solver algorithms are usually chosen to solve numerical models of large complex engineering systems. Numerical preconditioning can be used improve the convergence by applying a transformation to the original linear system that reduces the condition number, making it more amenable to numerical computation. A well-designed preconditioner can significantly reduce the number of iterations needed to solve a linear system of equations, leading to faster and more efficient numerical algorithms. Preconditioning techniques are widely used in various fields of science and engineering, such as computational fluid dynamics, finite element analysis, and optimization, among others. Especially in the field of uncertainty quantification efficient solving strategies are essential. Adaptive preconditioning is a technique used in numerical analysis to adjust the preconditioner used in an iterative solver during the solution process. The idea behind adaptive preconditioning is to improve the convergence of the iterative method by dynamically changing the preconditioner based on the current state of the solver. This approach can be particularly effective in situations where the characteristics of the linear system of equations change during the solution process, such as in nonlinear problems or problems with varying input parameters. Adaptive preconditioners can be implemented in several ways. One approach is to use a fixed set of preconditioners, each designed to work well for a specific range of problem parameters. The solver can then switch between the different preconditioners as needed during the solution process. Another approach is to modify the preconditioner directly based on information obtained during the iteration process, such as estimates of the eigenvalues of the system or the residual norms. These ideas can be used to enhance the performance of solving numerical models under polymorphic uncertainty where system parameters are described by different uncertainty models ranging from standard probability theory to polymorphic approaches. In the scope of uncertainty quantification the calculation of a certain number of samples of the numerical system is necessary to approximate the system's behavior. In this study, adaptive preconditioning is used to adjust the preconditioner to the sampled sets of the system's input parameters of a numerical system.

PP 1962: Non smooth and complementarity-based distributed parameter systems

Organizer(s): **Hintermüller, Michael** *(WIAS Berlin)*

PP 1962-01: Non smooth and complementarity-based distributed parameter systems

Date: May 31, 2023 14:00-16:00
Room: HSZ/204

Shape optimization in the Lipschitz topology with the ADMM method

Deckelnick, Klaus *(Otto-von-Guericke-Universität Magdeburg)*
Herbert, Philip *(Heriot-Watt University, Edinburgh)*
Hinze, Michael *(Universität Koblenz, Germany)*

14:00

We present a general shape optimisation framework based on the method of mappings in the Lipschitz topology. We propose steepest descent and Newton-like minimisation algorithms for the numerical solution of the respective shape optimisation problems. Our work is built upon previous work of the authors in (Deckelnick, Herbert, and Hinze, ESAIM: COCV 28 (2022)), where a Lipschitz framework for star-shaped domains is proposed. To illustrate our approach we present a selection of PDE constrained shape optimisation problems and compare our findings to results from so far classical Hilbert space methods and recent p-approximations.

PP 2020: Cyclic deterioration of high-performance concrete in an experimental-virtual lab

Organizer(s): **Storm, Johannes** *(TU Dresden)*
Aldakheel, Fadi *(Leibniz Universität Hannover)*

PP 2020-01: Cyclic deterioration of high-performance concrete in an experimental-virtual lab

Date: June 1, 2023 08:30-10:30
Room: HSZ/204

High-speed fatigue testing of High-Performance Concretes and parallel characterization using Dynamic Mechanical Analysis (DMA)

Madadi Varzaneh, Hamid Reza *(Institute of Applied Mechanics, University of Stuttgart, Germany)* 08:30
Steeb, Holger *(Institute of Applied Mechanics, University of Stuttgart, Germany)*

Due to cyclic load, fatigue affects brittle materials like (ultra) High-Performance Concrete (UHPC) used in marine and civil structures, resulting in unexpected failures. Additionally, in order to analyze mechanical properties of materials, understanding how materials respond to different frequencies is crucial for industrial designers. When a material is subjected to more fatigue cycles, its mechanical properties undergo changes. To extract material's properties under fatigue load at a specific cyclic speed, It is necessary to obtain the mechanical response of the material at the same frequency speed. Cyclic load tests are conducted to determine how fatigue affects the material and the number of cycles it will take to fail is experimentally determined. The problem with such tests is that they are potentially expensive, i.e., it could take a long time since the number of loading cycles can be extremely high. Moreover, it is not possible to observe the evolution of (micro-)cracks within the different damage phases of cycling tests. It is also challenging to characterize the material's small-strain stiffness evolution. This research aims to investigate the use of high-frequency excitation with a (large amplitude) dynamic mechanical testing (DMT) for the High Cycle Fatigue experiments and also in-parallel extraction of material properties with a (low amplitude) Dynamic Mechanical Analysis (DMA). The test setup applies excitation using high-voltage piezoelectric actuators and then the failure modes of the material will be examined. The excitation frequency for the fatigue test is between 10 and 200 cycles per second which allow for reducing the experimental investigation time to failure. Further, it allows investigation of the effect of frequency on the number of cycles to failure. In addition, the (rate-dependent) complex mechanical properties of the materials in tangential space are obtained in frequency between 0.01 Hz to 1000 Hz using direct measurement with DMA method; while, the observed mechanical properties of these materials change with increasing frequency. In the case of materials' behavior, by increasing the frequency, Young's modulus increases and Poisson's ratio decreases. Experimental fatigue results will be presented for (U)-HPC and Berea sandstone samples. Harmonic experimental data include (direct) strain measurements in axial and circumferential directions as well as forces in axial directions. In addition, the resulting complex Young's modulus and evolving

damage-like “history” of HPC and Berea sandstone specimens will be shown.

Fatigue failure mechanism for concrete microstructure in fully saturated porous media

Noii, Nima *(Institute of Continuum Mechanics, Leibniz University Hannover, Germany)* 08:50
Aldakheel, Fadi *(Institute of Continuum Mechanics, Leibniz University Hannover, Germany)*
Abubakar Ali, Mohamed *(Institute of Building Materials Science, Leibniz University Hannover, Germany)*
Oneschkow, Nadja *(Institute of Building Materials Science, Leibniz University Hannover, Germany)*
Haist, Michael *(Institute of Building Materials Science, Leibniz University Hannover, Germany)*
Lohaus, Ludger *(Institute of Building Materials Science, Leibniz University Hannover, Germany)*
Wriggers, Peter *(Institute of Continuum Mechanics, Leibniz University Hannover, Germany)*

The fatigue behavior of concrete with high moisture content has become an important subject of interest with the expansion of offshore wind energy systems. Investigations in the literature indicated that the number of cycles to failure significantly decreases with the increased moisture content in concrete. This work presents a novel variational phase-field model for modeling water-induced failure mechanisms due to the cyclic loading in concrete. As a key feature, the fatigue-induced fracture is formulated based on the accumulation of the bulk energy in time, and so a critical stress state (which indicates the crack initiation) will be drastically reduced [1].

These failure mechanisms are coupled to fluid flow, resulting in a Darcy-Biot-type hydro- mechanical model [2]. Here, the model employs a micromechanics-based theory for the description of specific fracture-driving state functions to model compression/shear regimes in concrete. As another important feature, the model includes a non-associative frictional plasticity law which is suitable for concrete [3, 4]. Numerical results confirmed that the fatigue effect results in the reduction of the crack resistance for the water-saturated case in comparison to the dry test. So the number of cycles to failure for both dry and fully saturated cases is analyzed over the degradation process.

Finally, the complete failure state of the specimen is further examined with an experimental observation to verify the proposed model. To do so, the influence of the loading frequency on the fatigue behavior of concrete has been investigated. This has been done for both dry and fully saturated media. We observed that the failure of high concrete moisture contents is more pronounced for lower load frequencies. This is further investigated through our proposed numerical formulation and validated with an experiment.

References

[1] K. Seleš, F. Aldakheel, Z. Tonkovic , J. Soric , P. Wriggers, A general phase-field model for fatigue failure in brittle and ductile solids, Com-put. Mech. 67 (2021) 1431-1452.
[2] N. Noii, A. Khodadadian, T. Wick, Bayesian inversion for anisotropic hydraulic phase-field fracture, Comput. Methods in Appl. Mech. Eng. 386 (2021) 114118.

[3] M. Abubakar Ali, C. Tomann, F. Aldakheel, M. Mahlbacher, N. Noii, N. Oneschkow, KH. Drake, L. Lohaus, P. Wriggers, M. Haist, Influence of moisture content and wet environment on the fatigue behavior of high-strength concrete, Materials 15 (2022) 1025.
[4] F. Aldakheel, A microscale model for concrete failure in poro-elasto-plastic media, Theor. Appl. Fract. Mech. 107 (2020) 102517.

Mesoscale Modeling Of High-performance Fiber-reinforced Concrete Under Monotonic And Cyclic Loading

Daadouch, Koussay *(Institute for Structural Mechanics, Faculty of Civil and Environmental Engineering, Ruhr-University Bochum, Germany)*
Gudžulić, Vladislav *(Institute for Structural Mechanics, Faculty of Civil and Environmental Engineering, Ruhr-University Bochum, Germany)*
Meschke, Günther *(Institute for Structural Mechanics, Faculty of Civil and Environmental Engineering, Ruhr-University Bochum, Germany)*

09:10

Concrete is the most widely used material in the construction industry. However, it also has a high environmental impact due to the energy-intensive cement production process. To alleviate this effect, high-performance and ultra-high-performance concrete and fiber reinforcement have been utilized to enhance durability and reduce material usage. However, better models and design techniques are necessary to leverage these advancements fully. This study explores the mechanical behavior of high-performance fiber-reinforced concrete. It presents a framework for creating numerical models of fiber-reinforced concrete at the mesoscale level based on virtual aggregate and fiber distributions or computed tomography images [1]. The fibers are modeled explicitly as elastoplastic Timoshenko beam elements, and the bond between the cement matrix and fibers is described using an elastoplastic bond-slip law. The fracture behavior is modeled discretely by zero-thickness interface elements equipped with a traction separation law. All these components are integrated into the open-source Finite Element program Kratos-Multiphysics. The capabilities of the model are demonstrated by reanalyzing experimental scenarios and comparing the results with available data [2]. This framework provides a comprehensive understanding of the behavior of high-performance fiber-reinforced concrete at small scales, which is crucial in developing better models and design techniques for the future.

[1] Holla V., Vu G., Timothy J. J., Diewald C., Gehlen C., Meschke G., *Computational generation of virtual concrete mesostructures*, Materials, Vol. 14, 2021.
[2] Schäfer N., Gudžulić V., Breitenbücher R., Meschke G., *Experimental and numerical investigations on high performance SFRC: Cyclic tensile loading and fatigue*, Materials, Vol. 14, 2021.

Phase-field modeling of failure behavior of reinforced ultra high performance concrete at low cycle fatigue

Pise, Mangesh *(Institut für Mechanik, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Universitätsstraße 11, 45141 Essen, Germany)* 09:30
Gebuhr, Gregor *(Chair for Construction Materials, Faculty of Architecture and Civil Engineering, Bergische Universität Wuppertal, Pauluskirchstraße 11, 42285, Wuppertal, Germany)*
Brands, Dominik *(Institut für Mechanik, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Universitätsstraße 11, 45141 Essen, Germany)*
Anders, Steffen *(Chair for Construction Materials, Faculty of Architecture and Civil Engineering, Bergische Universität Wuppertal, Pauluskirchstraße 11, 42285, Wuppertal, Germany)*
Schröder, Jörg *(Institut für Mechanik, Fakultät für Ingenieurwissenschaften, Universität Duisburg-Essen, Universitätsstraße 11, 45141 Essen, Germany)*

In the recent decades great research effort has been carried out which led to more efficient and stronger concrete types, e.g. high performance concrete (HPC) and ultra-high performance concrete (UHPC). They are rapidly emerging as promising materials in construction industries worldwide. HPCs are available in wide varieties of composition which make them different from classical concrete types. For example, steel fibers and short-wire fibers are usually added to ensure ductility in HPC and in UHPC, respectively. The fiber reinforcements provide a sufficient ductility by transmitting the stresses in concrete from matrix to the fibers during fracture. This process shows pronounced effect on the deterioration characteristics of concrete in cyclic flexural tests, see [2].

In this contribution, the aim is to investigate the influence of fiber's orientations and distribution on the overall material behavior of fiber reinforced UHPCs at low cyclic fatigue. A phenomenological material model is developed by combining the superposed models of transversal isotropic elasto-plasticity, see [1] and a continuum phase-field model of fracture in elasto-plastic material, cf. [3, 4]. Two different continuous stepwise linearly approximated degradation functions for the modeling of unsymmetric behavior of UHPC in tension and in compression are considered. The numerical model is calibrated using the experimental data and by simulating the typical uniaxial cyclic tests and three-point bending beam test at low cycle for pure UHPC. Three-point bending beam tests at low cycle for reinforced UHPCs with different fiber contents and orientations are simulated. To incorporate the different distributions and orientations of reinforced fibers different orientation distribution functions (ODF) are constructed and implemented. The degradation of residual stiffness is calculated using experimental and numerical results and compared to validate the accuracy of the numerical results, see [4, 5].

References

[1] J. P. Boehler. Applications of tensor functions in solid mechanics. CISM, 292, Springer, Vienna, 1987.

[2] K. Elsmeier, J. Hümme, N. Oneschkow and L. Lohaus. Prüftechnische Einflüsse auf das Ermüdungsverhalten hochfester feinkörninger Vergussbetone. Beton- und Stahlbetonbau, 111:233-240, 2016.

[3] C. Miehe, F. Aldakheel, and A. Raina. Phase-field modeling of ductile fracture at finite

strains: A variational gradient-extended plasticity-damage theory. International Journal of Plasticity, 84:1-32, 2016.
[4] M. Pise, D. Brands, J. Schröder, G. Gebuhr, S. Anders. Phenomenological material model for damage in steel-fiber reinforced high performance concrete during low cycle fatigue . Proceedings in Applied Mathematics and Mechanics, 22:e202200236, 2022.
[5] G. Gebuhr, M. Pise, S. Anders, D. Brands, J. Schröder. Damage evolution of steel fiber reinforced high performance concrete in low-cycle flexural fatigue: numerical modeling and experimental validation. Materials, 15:1179, 2022.

Modelling of Overload Effects on Fatigue Behaviour via Representative Crack Elements

Storm, Johannes *(Technische Universität Dresden, Germany, Institute for Structural Analysis)*
Kaliske, Michael *(Technische Universität Dresden, Germany, Institute for Structural Analysis)*

09:50

The energetic description of a crack dates back to Griffith, who has related the required energy to create a crack increment to the available potential energy in the system. Two regularisations for this problem are under strong developed and are applied to brittle fracture, namely phase-field fracture [1] and eigenfracture [2]. The authors have derived efficient numerical solution schemes in the context of phase-field fracture [3] and eigenfracture [4] for the realistic prediction of crack deformation by means of Representative Crack Models. The prediction of the crack state (opened/closed) and the forces, which can be transferred through a crack, are essential for the post-fracture behaviour but also for the calculation of the potential energy available to drive the crack.

In this talk, we apply the framework to the simulation of fatigue material behaviour at cyclic loading. The effect of overloads is investigated for elasto-plastic materials, which slow down the crack propagation through an interaction of the plastic zone with the crack tip field.

[1] G. Francfort and J. Marigo, Journal of the Mechanics and Physics of Solids 46, 1319-1342 (1998).
[2] B. Schmidt, F. Fraternali, and M. Ortiz, Multiscale Modeling & Simulation 7, 1237-1266 (2009).
[3] J. Storm, D. Supriatna, and M. Kaliske, International Journal for Numerical Methods in Engineering 121, 779-805 (2020).
[4] J. Storm, A. Qinami, and M. Kaliske, Mechanics Research Communications 116, 103747 (2021).

PP 2256: Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials

Organizer(s): **Mosler, Jörn** *(TU Dortmund)*
Schmidt, Bernd *(University of Augsburg)*

PP 2256-01: Variational Methods for Predicting Complex Phenomena in Engineering Structures and Materials

Date: June 1, 2023 16:00-18:00
Room: HSZ/204

Approximation schemes for energies of prescribed fracture geometry

Wozniak, Piotr *(University of Münster, Germany)* 16:00

One perspective in the study of metamaterials concerns the question of designing high-contrast composites with desired effective properties. More precisely one may contemplate possible microstructures of simplistic patterns which in the macroscopic scale would give rise to ductile materials favouring fracture only in accord with prescribed directions. In terms of variational modelling this objective is articulated as the asymptotic analysis, or Gamma convergence, of surface-degenerate Mumford-Shah energies. In this talk we propose and discuss the model functional set in the realm of SBV -type spaces along with the determining microgeometry. Within such formulations a general displacement field may admit highly irregular cracks in the reference domain. Therefore In order to rigorously derive the homogenised limit it is essential to come up with density techniques that approximate the surface energy by more regular competitors. We are going to point out some key challenges in proving the desired Gamma convergence and report on partial progress on the matter.

Balanced-Viscosity solutions for a Penrose-Fife phase-field model with friction

Liero, Matthias *(Weierstrass Institute Berlin, Germany)* 16:20
Mielke, Alexander *(Weierstrass Institute Berlin, Germany; Humboldt-Universität zu Berlin)*
Pelech, Petr *(Charles University)*

We consider an adapted Penrose-Fife model for a phase-field variable and the internal energy, where the phase transformation is an activated process. The latter is described via a rate-independent contribution with respect to the rate of the phase-field variable. We discuss the existence of solutions exploiting the gradient-flow structure of the equations and present results on the derivation of the effective evolution in the case of slow loading regimes using the notion of balanced-viscosity solutions. While the complexity of the system is not too heavy, there remain intrinsic difficulties, like the non-uniform convexity and the weak growth of the negative entropy with respect to the internal energy allowing for the formation of singular measures.

Modeling and Simulation of Thin Sheet Folding

Bartels, Sören *(University of Freiburg, Germany)* 16:40

The folding of a thin elastic sheet along a curved arc has various applications including the construction of bistable devices. We discuss the derivation of a plate model from three-dimensional hyperelasticity and rigidity properties of admissible deformations and minimizers. The numerical solution is based on an isoparametric discontinuous Galerkin finite element method that provides a suitable geometric approximation of the folding arc. Error estimates are presented for a linearized version of the model problem. This is joint work with Andrea Bonito (Texas A&M), Peter Hornung (TU Dresden) and Philipp Tscherner (U Freiburg).

Perspectives for homogenization on randomly perforated domains

Heida, Martin *(WIAS Berlin, Germany)*
Vu, Duc *(WIAS Berlin, Germany)*
Jahnel, Benedikt *(WIAS Berlin, Germany)* 17:00

We look at homogenization problems on randomly perforated domains from the geometric point of view: In many models the randomness creates geometries that are locally Lipschitz and harmless, but become arbitrarily bad on large scales. We provide two different points of view how the effect of the large scale irregularities might be controlled in the homogenization process: One is using wieghts on averaged local quantities, the other is using a sequence of global regularization operators.

Regularity questions in geometrically nonlinear Cosserat elasticity

Gastel, Andreas *(Universität Duisburg-Essen, Germany)*
Hüsken, Vanessa *(Universität Duisburg-Essen, Germany)* 17:20

We consider Cosserat-type micropolar elasticity models which are nonlinear with respect to the rotational part of the energy. The system of Euler-Lagrange equations is that of harmonic maps to SO(3) coupled with another elliptic equation. We discuss theorems on the regularity of solutions as well as the construction of singular solutions. Both sorts of behaviour resemble those observed for harmonic maps. We will also comment on aspects of the models where the adaptation of harmonic maps methods should be difficult.

Scaling laws for multi-well nucleation problems

Tribuzio, Antonio *(Heidelberg Univesrity, Germany)*
Rüland, Angkana *(Heidelberg Univesrity, Germany)* 17:40

In this talk, we study scaling laws for nulceation problems which are motivated by models for shape-memory alloys. More precisely, we discuss optimal energy scaling of inclusions of a phase with several variants (martensite) inside a parent phase (austenite), for various model problems in two and three dimensions. The energy term is given by a singularly-perturbed multi-well elastic energy (without gauge invariances). We provide scaling results in the volume and the singular perturbation parameter for settings in which the surrounding parent phase is in the first-, the second- and the third-order lamination-convex hull of the wells of the "martensite phase". Furthermore, we provide a corresponding result for the setting of an infinite-order laminate which arises in the context of the Tartar square.

PP 2298: Theoretical Foundations of Deep Learning

Organizer(s): **Kutyniok, Gitta** *(LMU Munich)*
Thesing, Laura *(LMU Munich)*

PP 2298-01: Theoretical Foundations of Deep Learning

Date: June 2, 2023 08:30-10:30
Room: HSZ/204

Curse-of-Dimensionality-free Approximations of Optimal Value Functions with Neural Networks under a Decaying Sensitivity Assumption

Grüne, Lars *(University Bayreuth, Germany)* 08:30
Sperl, Mario *(University Bayreuth, Germany)*

It is known that neural networks are capable of overcoming the curse of dimensionality for approximating functions with certain beneficial structures, e.g. separable functions. In this talk, we discuss the use of neural networks for solving optimal control problems by computing a separable approximation of the optimal value function. We consider an interconnected control system that is represented by a directed graph. In order to establish the existence of a separable approximation of the optimal value function, we rely on a decay property of the sensitivity between nodes with their graph-distance. In particular, we demonstrate how such a decay property can be used to construct a separable approximation of the optimal value function by considering graph-neighborhoods of the single subsystems. Moreover, conditions under which a decay of sensitivity has been established in the literature are discussed. Further, we present a neural network architecture that can be used to perform the corresponding computation.

Implicit bias of gradient descent for learning linear neural networks

Rauhut, Holger *(RWTH Aachen University, Germany)* 08:50

Deep neural networks are usually trained by minimizing a non-convex loss functional via (stochastic) gradient descent methods. A puzzling empirical observation is that learning neural networks with a number of parameters exceeding the number of training examples often leads to zero loss, i.e., the network exactly interpolates the data. Nevertheless, it generalizes very well to unseen data, which is in stark contrast to intuition from classical statistics which would predict a scenario of overfitting. A current working hypothesis is that the chosen optimization algorithm has a significant influence on the selection of the learned network. In fact, in this overparameterized context there are many global minimizers so that the optimization method induces an implicit bias on the computed solution. It seems that gradient descent methods and their stochastic variants favor networks of low complexity (in a suitable sense to be understood), and, hence, appear to be very well suited for large classes of real data. Initial attempts in understanding the implicit bias phenomen considers the simplified setting of linear networks, i.e., (deep) factorizations of matrices. This has revealed a surprising relation to the field of low rank matrix recovery (a variant of compressive sensing) in the sense that gradient descent favors low rank matrices in certain situations. Moreover, restricting further

to diagonal matrices, or equivalently factorizing the entries of a vector to be recovered, shows connection to compressive sensing and l1-minimization. After giving a general introduction to these topics, the talk will concentrate on results by the speaker on the convergence of gradient flows and gradient descent for learning linear neural networks and on the implicit bias towards low rank and sparse solutions.

Improved Representation Learning Through Tensorized Autoencoders

Esser, Pascal Mattia *(Technical University of Munich, Germany)*
Mukherjee, Satyaki *(Technical University of Munich, Germany)*
Sabanayagam, Mahalakshmi *(Technical University of Munich, Germany)*
Ghoshdastidar, Debarghya *(Technical University of Munich, Germany)*

09:10

The central question in representation learning is what constitutes a good or meaningful representation. In this work we argue that if we consider data with inherent cluster structures, where clusters can be characterized through different means and covariances, those data structures should be represented in the embedding as well. While Autoencoders (AE) are widely used in practice for unsupervised representation learning, they do not fulfil the above condition on the embedding as they obtain a single representation of the data. To overcome this we propose a meta-algorithm that can be used to extend an arbitrary AE architecture to a tensorized version (TAE) that allows for learning cluster-specific embeddings while simultaneously learning the cluster assignment. For the linear setting we prove that TAE can recover the principle components of the different clusters in contrast to principle component of the entire data recovered by a standard AE. We validated this on planted models and for general, non-linear and convolutional AEs we empirically illustrate that tensorizing the AE is beneficial in clustering and de-noising tasks.

On the ELBO of Probabilistic Generative Models and Its Equality to Entropy Sums at Convergence

Lücke, Jörg *(University of Oldenburg, Germany)*
Damm, Simon *(Ruhr-University Bochum, Germany)*
Forster, Dennis *(Frankfurt University of Applied Science, Germany)*
Velychko, Dmytro *(University of Oldenburg, Germany)*
Fischer, Asja *(Ruhr-University Bochum, Germany)*
Dai, Zhenwen *(Spotify, London, UK)*

09:30

The optimization of probabilistic generative models is a central task for unsupervised learning, and such an optimization often seeks model parameters that maximize the data likelihood given a model of interest. However, for most generative models (including most deep generative models) the likelihood is not analytically tractable. A very prominent and successful approximation strategy has therefore been to instead optimize a variational lower bound (a.k.a. evidence lower bound or ELBO) of the log-likelihood. While optimization is facilitated in this way, the ELBO, e.g., for deep generative models, remains analytically intractable, which motivates further approximations to enable efficient optimization. When learning algorithms optimize the ELBO, they change model parameters usually until they have converged to values close to a stationary point of the learning dynamics. In the here presented line of research,

we analyze the stationary points of learning algorithms that are based on the ELBO objective. The main result we discuss is that (for a very large class of generative models) the ELBO becomes equal to a sum of entropies at all stationary points (i.e., at all points learning converges to). For standard machine learning models with one set of latents and one set of observed variables, the sum consists of three entropies: (A) the (average) entropy of the variational distributions, (B) the negative entropy of the model's prior distribution, and (C) the (expected) negative entropy of the observable distributions. The obtained result applies under realistic conditions including: finite numbers of data points, at any stationary point (including saddle points), and for any family of (well behaved) variational distributions. The class of generative models for which we discuss the equality to entropy sums contains well-known generative models such as Sigmoid Belief Networks, probabilistic PCA, most mixture models as well as standard variational autoencoders (VAEs). VAEs range amongst the most prominent and successful deep generative models. While their ELBO objective is (except of linear boundary cases) considered analytically intractable, we show that the ELBO values can be computed in closed-form at all stationary points. Furthermore, we present a numerical analysis which is part of a contribution recently presented at AISTATS (Damm et al., 2023). The analysis verifies convergence to entropy sums for VAEs, and shows that closed-form ELBO expressions match the original ELBOs well in the vicinity of stationary points. Finally, we discuss properties of the optimization landscape that can be derived from the presented results, and close with an outlook.

Robustness of Low Rank Matrix Recovery under Adversarial Noise

Kostin, Julia *(Technische Universität München, Germany)*
Krahmer, Felix *(Technische Universität München, Germany)*
Stöger, Dominik *(Katholische Universität Eichstätt-Ingolstadt)*

09:50

Machine learning methods, in particular end-to-end neural networks, have recently achieved remarkable success in solving linear inverse problems such as image deblurring or super-resolution. However, a question particularly relevant for medical applications (e.g. MRI) remains whether their performance remains stable under small adversarial perturbations of the input. As a first step towards proving robustness of neural networks for inverse problems, we study the problem of recovering a low-rank matrix from a limited set of randomized measurements corrupted by bounded, possibly adversarial noise. Low-rank matrix recovery includes problems such as blind deconvolution and matrix completion. Wide use of the nuclear norm minimization heuristic instead of rank minimization has lead to a series of theoretical recovery guarantees for low-rank recovery problems in the last two decades. In particular, in the absence of noise, exact recovery with high probability has been established for sufficiently incoherent signals. However, in presence of bounded, possibly adversarial additive noise, stability of low-rank matrix recovery remains much less clear. In particular, existing reconstruction error bounds involve large dimensional factors and therefore fail to explain the empirical evidence for dimension-independent robustness of nuclear norm minimization. Moreover, recently theoretical evidence has emerged that low-rank matrix recovery can be unstable if the noise level is sufficiently small. In this work, we develop new recovery error

guarantees for the settings of blind deconvolution and matrix completion with adversarial noise which depend on the noise level and are thus consistent with existing counterexamples. We end our discussion with the interesting question whether similar unstable behavior can be rigorously demonstrated for neural networks utilized for low-rank matrix recovery and similar linear inverse problems.

PP 2311: Robuste Kopplung kontinuumsbiomechanischer in silico Modelle für aktive biologische Systeme als Vorstufe klinischer Applikationen – Co-Design von Modellierung, Numerik und Nutzbarkeit

Organizer(s): **Ricken, Tim** *(University of Stuttgart)*
Röhrle, Oliver *(University of Stuttgart)*

PP 2311-01: Robuste Kopplung kontinuumsbiomechanischer in silico Modelle für aktive biologische Systeme als Vorstufe klinischer Applikationen – Co-Design von Modellierung, Numerik und Nutzbarkeit

Date: June 2, 2023 11:00-13:00
Room: HSZ/204

Simulation Supported Liver Assessment for Donor Organs (SimLivA) - Continuum-Biomechanical Modeling for Staging of Ischemia Reperfusion Injury During Liver Transplantation

Mandl, Luis *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Germany)*
Gerhäusser, Steffen *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Germany)*
Lambers, Lena *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Germany; Experimental Transplantation Surgery, Department of General, Visceral and Vascular Surgery, Jena University Hospital, Germany)*
König, Matthias *(Institute for Theoretical Biology, Humboldt University Berlin, Germany)*
Tautenhahn, Hans-Michael *(Experimental Transplantation Surgery, Department of General, Visceral and Vascular Surgery, Jena University Hospital, Germany; Department of General, Visceral and Vascular Surgery, Jena University Hospital, Germany)*
Dahmen, Uta *(Experimental Transplantation Surgery, Department of General, Visceral and Vascular Surgery, Jena University Hospital, Germany)*
Ricken, Tim *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Faculty of Aerospace Engineering and Geodesy, University of Stuttgart, Germany)*

11:00

Liver transplantation is the only curative treatment option for acute and chronic end-stage liver disease. Demographic change and western lifestyle result in an increasing number of elderly multi-morbid potential recipients and donors. Liver grafts from such donors, so-called marginal liver grafts, are often affected by hepatic steatosis compromising the quality of the donor organ substantially. One reason for this is the alteration of the tissue structure, resulting in an impaired perfusion, which in turn affects hepatic metabolism and organ function. In the case of a marginal graft, the surgeon is faced with the clinical decision to either accept or reject the organ, significantly increasing the postoperative risk for the recipient or increasing the risk of death on the waiting list, respectively. Two major challenges for marginal grafts

are the storage between procurement of the organ and transplantation (cold ischemia time) and damage after reperfusion, the so-called ischemia reperfusion injury (IRI).

For this purpose, we describe the functional liver units, the liver lobules, as a homogenized porous medium and model this with the theory of porous media (TPM, cf. [1]). Considering an anisotropic blood flow and by coupling the metabolic processes at the cellular level, a poroelastic multiphase and multiscale function-perfusion model is thereby obtained (cf. [2]). This approach combines partial differential equations (PDE) on the lobular scale with ordinary differential equations (ODE) on the cellular scale resulting in a PDE-ODE coupling. At the lobular scale, we consider healthy liver tissue, necrotic tissue, and fat as solid phases, while blood is represented as a fluid phase. In addition, all phases may also contain solutes that are involved in cellular processes such as metabolism. Based on this, the energy balance and cell death or functionality of each cell can be modeled on the cellular scale using systems biology models. Thus, the ischemic damage under nutrient depletion can be described, which in turn affects the perfusion at the lobular scale. Animal and human data will be used to parameterize and validate the model. In addition, a proof-of-concept study for clinical applicability will be performed. Such a model, which takes into account the interplay between the mechanical properties of the graft, the hepatic perfusion, and the affected metabolism, could facilitate clinical decision making and is urgently needed cf. 3.

[1] Ehlers,W. Foundations of multiphasic and porous materials(2002)
[2] Ricken,T., et al. BMMB(2015) 14:515-536
[3] Christ,B.,[...],Lambers,L.,[...]Ricken,T.,et al. Frontiers in Physiology(2021)12

Bifurcations and patterns in a cell-based mathematical model for meniscus tissue regeneration

Mohan, Nishith *(Felix-Klein-Zentrum für Mathematik, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany)*
Surulescu, Christina *(Felix-Klein-Zentrum für Mathematik, Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany)*

11:20

We propose a model for the dynamics of adipose derived stem cells (ADSCs) and chondrocytes responding to hyaluron concentration signals. Thereby, ADSCs and chondrocytes are motile, while hyaluron is fixed on the artificial scaffold in which the cells are embedded. The movement of ADSCs is governed by haptotaxis and diffusion. Haptotaxis represents the situation where cells bias their migration towards the gradient of a non-diffusible component (here hyaluron). The chondrocytes are assumed to be diffusive, but their motility does not affect the movement of ADSCs. The equations characterizing the dynamics of the two cell populations are of reaction-diffusion(-taxis) type, while hyaluron concentration evolves according to an ODE. A mathematical analysis showed that the proposed mathematical model can exhibit bifurcation, instability, and pattern formation. The patterning behavior was also investigated by way of simulations. The study aims to understand the rich dynamics associated with PDE-ODE coupled systems describing processes involved in meniscus regeneration.

Data Sharing for Collaborative Modeling and Simulation Research

Villota-Narvaez, Yesid *(Institute for Modeling and Simulation of Biomechanical Systems, University of Stuttgart)*
Röhrle, Oliver *(Institute for Modeling and Simulation of Biomechanical Systems, University of Stuttgart)*

11:40

The process of creating accurate and reliable biomechanical models and simulations requires the integration of data from geometric shapes, material properties, kinematic movement, and physiological factors of biological systems, which can be obtained through various sources and techniques. This integration demands access to information and collaboration between researchers and institutions and makes data sharing crucial in the context of modeling and simulation research. A structured approach is required to attend to the complexity of simulation data, and the variety of user needs and criteria. This approach follows the FAIR principles of findability, accessibility, interoperability, and reusability, and provides a framework for data sharing that could be used to improve the data-sharing process. These principles also promote the responsible use of research data and provide a roadmap for making data more useful for the scientific community and society. By following the FAIR principles, data sharing: (1) enables the exchange of data between different simulation tools, models, and software platforms; (2) facilitates the creation of safeguards and standards to protect the privacy and security of shared data; (3) promotes transparency and increases the reproducibility of research; (4) allows for the sharing of data sets to create more accurate and reliable simulations; and (5) facilitates collaboration between research groups and institutions. This contribution outlines the general steps for sharing research data, which include preparing the data, selecting an appropriate data-sharing platform, determining access and sharing options, uploading and describing the data, and publishing and citing the data. Despite all the benefits of data sharing, the decision to share research data should be based on a balance between the potential benefits to scientific knowledge, the protection of individual privacy and security, any legal or ethical constraints, and the nature of the data.

Modeling Drug Diffusion and Smooth Muscle Response in Arteries

Nurani Ramesh, Sharan *(Ruhr-Universität Bochum)*
Saßmannshausen, Lea *(Universität zu Köln)*
Uhlmann, Klemens *(Ruhr-Universität Bochum)*
Heinlein, Alexander *(Technische Universiteit Delft)*
Rheinbach, Oliver *(Technische Universität Bergakademie Freiberg)*
Klawonn, Axel *(Universität zu Köln)*
Balzani, Daniel *(Ruhr-Universität Bochum)*

12:00

Antihypertensive drugs are regularly used to treat high blood pressure. Certain combinations of drugs, however, have been linked to ischemic events [1]. To better understand the physics of plaque disruption under medicinal influence, we numerically simulate healthy and atherosclerotic arteries. This necessitates an accurate description of drug dispersion and an appropriate material model for the arterial wall. The stretch dependent smooth muscle model by Uhlmann and Balzani [2] is extended to include pharmacological effects. The coupled deformation-diffusion problem is then solved using the finite element based software

FEDDLib [3] and Schwarz preconditioners from the Trilinos [4] package FROSch [5]. These preconditioners include highly-scalable parallel GDSW (generalized Dryja-Smith-Widlund) preconditioners [6] which are also applicable to fluid-structure interaction problems. Simulation results for a simple arterial wall section will be presented and discussed.

[1] Howard, George, et al. "Is blood pressure control for stroke prevention the correct goal? The lost opportunity of preventing hypertension." Stroke 46.6 (2015): 1595-1600.
[2] Uhlmann, K., Balzani, D. (in press), "Chemo-mechanical modeling of vascular smooth muscle cells for the simulation of arterial walls under changing blood pressure", In Biomechanics and Modeling in Mechanobiology. Springer
[3] FEDDLib (Finite Element and Domain Decomposition Library). Github repository `https://github.com/FEDDLib/FEDDLib.2022`.
[4] The Trilinos Project Team. The Trilinos Project Website `https://trilinos.github.io`. 2022.
[5] A. Heinlein, A. Klawonn, S. Rajamanickam, and O. Rheinbach. "FROSch: A Fast and Robust Overlapping Schwarz domain decomposition preconditioner based on Xpetra in Trilinos." In Domain Decomposition Methods in Science and Engineering XXV, pages 176-184, Cham, 2020. Springer International Publishing.
[6] A. Heinlein, C. Hochmuth, and A. Klawonn. "Monolithic overlapping Schwarz domain decomposition methods with GDSW coarse spaces for incompressible fluid flow problems." SIAM Journal on Scientific Computing, 41(4):C291-C316, 2019.

Multiscale analysis of intracranial arteriovenous malformations including realistic nidus segmentation and patient-specific hemodynamics

Stahl, Janneck *(Research Campus STIMULATE, University of Magdeburg, Germany; Department of Fluid Dynamics and Technical Flows, University of Magdeburg, Germany)*
Korte, Jana *(Research Campus STIMULATE, University of Magdeburg, Germany; Department of Fluid Dynamics and Technical Flows, University of Magdeburg, Germany)*
Spitz, Lena *(Research Campus STIMULATE, University of Magdeburg, Germany; Department of Simulation and Graphics, University of Magdeburg, Germany)*
Behme, Daniel *(Research Campus STIMULATE, University of Magdeburg, Germany; Department of Neuroradiology, University Hospital of Magdeburg, Germany)*
Kaneko, Naoki *(Department of Radiological Sciences, University of California, Los Angeles, USA)*
Alaraj, Ali *(Department of Neurosurgery, University of Illinois, Chicago, USA)*
Saalfeld, Sylvia *(Research Campus STIMULATE, University of Magdeburg, Germany; Department of Simulation and Graphics, University of Magdeburg, Germany)*
Berg, Philipp *(Research Campus STIMULATE, University of Magdeburg, Germany; Department of Medical Engineering, University of Magdeburg, Germany)*

12:20

Intracranial arteriovenous malformations (AVMs) are challenging neurovascular pathologies. With an abnormal tangle-like blood vessel network called nidus they are directly connecting the intracranial arteries and veins bypassing the capillary system. AVMs exhibit increased blood flow velocities in the feeding arteries and the draining veins, which can lead to complex hemodynamic patterns promoting possible rupture of the vessel walls.

Since AVMs connect two vascular systems, a deeper understanding of the complex vasculature as well as the blood flow patterns inside these structures are necessary. Especially when evaluating possible treatment options, precise comprehension of the vascular connections is required. Multiple imaging modalities are needed to acquire both vasculatures connected by the AVM nidus to resolve large scale morphologic information. Furthermore, a detailed flow-related analysis of the individual impact of multiple feeding arteries and draining veins on the nidus are not available yet.

This study aims to model large scale AVMs based on multimodal imaging. In addition to 3D digital subtraction angiography (3D DSA) and magnetic resonance angiography (MRA) data, especially magnetic resonance venography (MRV) data is used to capture the overall vasculature. 3D model extractions using threshold-based segmentation methods and extensive post-processing allows for the generation of realistic vascular models. In particular for generating large scale 3D models, registration of the partial segmentation data is conducted using a rigid body registration method. Based on the extracted 3D models, image-based blood flow simulations are conducted with a finite-volume based solver. By virtually adjusting the AVM models a simplified embolization treatment was simulated to analyze its hemodynamic influence on the connected vascular structures.

The results comprise complex large scale AVM models which are pathologically connecting the two vascular systems of the brain. Detailed hemodynamic information are obtained by patient-specific blood flow simulations. Qualitative and quantitative centerline-based hemodynamic evaluations provide physicians with individual options for assessing parameter changes in the overall vascular environment. Furthermore, adjusted 3D models virtually recreated different treatment stages, which allows pre-interventional therapy planning. This is further supported by an analysis of the hemodynamic impact of individual feeding arteries.

The proposed workflow allows in-depth insights into hemodynamic characteristics of patient-specific AVMs that are not available by conventional imaging. Thus, it sets the base to support risk assessment and treatment planning in clinical practice.

Statistical mechanics approach to neuron excitation

Werneck, Linda *(University of Stuttgart, Germany)* 12:40
Yildiz, Erdost *(Max Planck Institute for Intelligent Systems, Germany)*
Keip, Marc-Andre *(University of Stuttgart, Germany)*
Ortiz, Michael *(Caltech, USA)*

In the context of ultrasound neuromodulation, mechanosensitive ion channels of biomembranes play a major role. Wiggins and Phillips [1] describe the activation of such channels in bacteria as statistical events that depend on strain acting on the membrane.

In the present contribution, a two-state model for opening and closing of human neuron channels under strain is presented. The free energy of the membrane-channel-system is considered in form of conformational probabilities in a statistical mechanics framework. Further, the effect of the mechanical stimulation on the action potential is discussed and insights on neuronal response are given.

[1] Wiggins, P.A., Phillips, R. (2003). Analytic models for mechanotransduction: Gating a mechanosensitive channel. Proceedings of the National Academy of Sciences of the United States of America 101, 4071 - 4076.

PP 2353: Daring More Intelligence – Design Assistants in Mechanics and Dynamics

Organizer(s): **Eberhard, Peter** *(University of Stuttgart)*

PP 2353-01: Daring More Intelligence – Design Assistants in Mechanics and Dynamics

Date: May 31, 2023 08:30-09:30
Room: HSZ/204

Approaches for the approximation of acoustic models by deep learning

Schultz, Julius *(TU Braunschweig, Germany)* 08:30
van Delden, Jan *(University of Göttingen, Germany)*
Blech, Christopher *(TU Braunschweig, Germany)*
Langer, Sabine C. *(TU Braunschweig, Germany)*
Lüddecke, Timo *(University of Göttingen, Germany)*

Noise prevention in product development is becoming more and more important due to health effects and comfort restrictions. In the product development process costly and time-consuming simulations are carried out over parameter spaces using models in order to find quiet product designs. The solution of dynamic systems is limited in their maximum frequency and the size of the parameter space, even with today's computing capacities. For an efficient search within the parameter space, the substitution of high-fidelity models by machine learning approaches is subject of research. The major objective of the project "Design to Acoustics Through Deep Learning" within the DFG Priority Programme 2353 is a contribution to a paradigm shift in vibroacoustic design by generative deep learning using neural networks. In this contribution, an overview on the project's design concepts is given and first results on the approximation of academic examples are shown.

As a first step, we will teach a neural network to efficiently approximate the mapping from design parameters to frequency spectrums at different locations. Furthermore, we will investigate to which degree such representations can generalise outside of the training parameter range. To this end, useful inductive biases will be studied and integrated into the neural network.

In a second phase, we will make use of previously trained networks to generate suggestions of how to alter the design space for desirable properties (e.g. decreased perceived loudness). An engineering approach is to optimize the design parameters to match desired outputs while freezing the network. As a second approach, we will employ a generative adversarial network (GAN) to generate proposals. Here the idea is to train a generator conditioned on a target output to predict the required design parameters for this output while a discriminator network tries to identify fake parameter/output pairs. Both can be trained jointly by competing against each other.

We recently started the first project phase by working on academic examples, which can be solved analytically. Here, we trained a network to predict the frequency response of a spring mass oscillator using a simple multi-layer perception (MLP). We find this simple model consisting of only a few layers to learn well. However, generalisation to out-of-training parameters

fails and motivates the need for incorporating better inductive biases.

Path planning and control of concentric tube continuum robots

Ding, Zhaoheng *(TU Ilmenau, Germany)*
Flaßkamp, Kathrin *(Saarland University, Germany)*
Hoffmann, Matthias K. *(Saarland University, Germany)*
Mühlenhoff, Julian *(TU Ilmenau, Germany)*
Sattel, Thomas *(TU Ilmenau, Germany)*

08:50

Concentric tube continuum robots provide interesting opportunities for novel surgical procedures, as, e.g., in stereotactic neurosurgery. For simulation, design optimization, and path planning, a system model needs to be found, which is challenging due to various nonlinear effects in the infinite-degree-of-freedom system and the corresponding optimal planning problem. Thus, we combine first-principle models with data-based techniques throughout the design process.

As a starting point, the Rucker model for concentric tubes [1] is considered. In [2,3], we use unsupervised learning methods to derive ellipsoidal obstacles from labeled MRI and CT data for the neurosurgery planning problem, which can then be solved by gradient-based nonlinear optimization. Recent work adds a feedback strategy to the toolchain. To compensate model inaccuracies that are caused by nonlinearities, such as friction, material hysteresis, and non-concentricity, feedback control for the concentric tube's tool-tip is added. For a concentric tube robot that allows automated steering, measurement data is collected by a photogrammetric system. Based on this, we amend the optimal-control output following the idea of iterative learning control. That is, we iteratively derive corrections to improve tool-tip position accuracy by using sensitivity-information from the model. This approach is evaluated in an experimental setup.

[1] Rucker, D.C. (2011). The mechanics of continuum robots: model-based sensing and control. PhD thesis, Vanderbilt University. http://hdl.handle.net/1803/14268
[2] Hackenberg, A., Worthmann, K., Pätz, T., Keiner, D., Oertel, J., Flaßkamp, K. (2021). Neurosurgery planning based on automated image recognition and optimal path design. at- Automatisierungstechnik 69(8), 708-721, De Gruyter.
[3] Hoffmann, M. K., Esterhuizen, W., Worthmann, K., Flaßkamp, K. (2022). Path Planning for Concentric Tube Robots: a Toolchain with Application to Stereotactic Neurosurgery, arXiv preprint https://arxiv.org/abs/2211.15206

Towards intelligent design assistants for planar multibody mechanisms

Röder, Benedict *(University of Stuttgart, Germany)*
Ebel, Henrik *(University of Stuttgart, Germany)*
Eberhard, Peter *(University of Stuttgart, Germany)*

09:10

General-purpose robots can perform a broad range of tasks but are usually rather heavy and expensive. In situations where only particular movements need to be executed, more efficient special-purpose robots can be employed. However, they typically require an expert to design the system based on manual inspection of simulations and empirical results. This procedure is not only time-consuming, but the outcome also depends on the expert's experience.

Hence, the design process stems from subjective criteria while only a limited number of structurally different mechanisms can be considered. In contrast, a design assistant can consider a broad range of mechanisms and leverage multi-objective optimization to retrieve optimal designs for the given task. This approach requires a mathematical formulation of objective performance criteria. The objective function also needs to take special care of infeasible configurations. Due to the systems being synthesized based on mathematical functions rather than individual experience, the assistant allows a more transparent development of optimal problem-specific mechanisms compared to the conventional process. Experts can then fine-tune and analyze the proposed designs to compose the final system. In this context, this contribution aims at optimizing a planar multibody mechanism design to reach individual target points or follow a prescribed trajectory. In particular, we do not only want to optimize the shape or topology of individual parts of the manipulator but the structure of the manipulator itself, i.e., how many bodies to use or where to place links. Thus, the developed method is employed on an atlas of different mechanism designs to detect the most suitable ones for the given task. We investigate if the framework should follow a parallelized brute-force approach for finding globally optimal mechanisms or use swarm optimization and genetic algorithms to reduce the search space and retrieve locally optimal designs.

Sections

S01: Multi-body dynamics

Organizer(s): **Ellermann, Katrin** *(TU Graz)*
Edelmann, Johannes *(TU Wien)*

Multibody dynamics enables the simulation of a wide variety of systems, all characterized by having multiple parts in relative motion with one another. Applications span from biological to engineering systems, requiring diverse capabilities which range from real-time simulation to high fidelity modeling of complex multidisciplinary systems. Goal of this mini-symposium is to present a view on the latest developments in models and advanced numerical methods in multibody dynamics. Focus is on techniques that enable applications to complex real-life problems.

S01-01: Multi-body dynamics

Date: May 31, 2023 14:00-16:00
Room: POT/351

An improved development process of production plants using digital twins with extended dynamic behavior in virtual commissioning.

Pfeifer, Denis *(Instite of Engineering and Computational Mechanics, University of Stuttgart, Germany; ISG Industrielle Steuerungstechnik GmbH, Stuttgart, Germany)*
Scheid, Jonas *(Instite of Engineering and Computational Mechanics, University of Stuttgart, Germany)*
Fehr, Jörg *(Instite of Engineering and Computational Mechanics, University of Stuttgart, Germany)*

14:00

Virtual commissioning (VC) is used today to check and optimize the quality of control programs using digital twins instead of the real plant, in addition VC reduces the commissioning time. The digital twin simulates the plant behavior and the control system is connected in a software- or hardware-in-the-loop simulation (HiLS / SiLS). The simulation focuses on accurately mapping the interface to the control system. In addition, the material flow is simulated with highly abstracted physics, while handling tasks and material removal are typically handled on a purely kinematic level. This superficial VC model depth is sufficient for certain types of plants to reduce their commissioning time and perform optimization of operating processes.

However, with the demand for higher plant performance while reducing energy consumption and development time, lightweight designs and modern control concepts are emerging. This requires the consideration of dynamic behavior, such as flexible deformation of components and thus the current simple modeling approaches, i.e. point masses and simplified impulse-based contact treatment using primitive collision shapes, are no longer sufficient. Therefore, it is necessary to include the dynamics, i.e. elastic multibody dynamics and Lagrangian-based contact treatment, of production plants in VC simulation and ultimately in control programming.

Besides the additional modeling effort and the technical hurdle to implement plant dynamics models in VC, this also increases the demand on the know-how of the VIBN engineer. This

represents an additional difficulty in times of shortage of skilled workers.

The solution presented here, therefore, follows the approach where the modeling of dynamics models is performed in domain-specific tools. Often, suitable dynamics models exist, e.g., from the mechanical design step. These models can be adapted for VC and exported as black-box models via standardized interfaces from the expert tools and integrated into the VC tool, where models are deployed in a co-simulation fashion. This procedure saves the renewed modeling by the VC engineer and allows easy and IP-protected use, in which only the parameters relevant to VC are disclosed.

This approach is validated by modeling an inverse pendulum as a flexible multibody system in expert tools and then integrating it into the VIBN simulation via the Functional Mock-Up Interface (FMI). This enables a virtual design of the control system.

The second example is a robot for palletizing processes, focusing on an agile lightweight solution at a competitive cost point. Here, a digital twin supports complete mechatronic development in the early development phase.

Energy Efficiency of a Bipedal Robot That Walks on Compliant Ground

Luo, Yinnan *(Karlsruhe Institute of Technology, Germany)* 14:40
Arbogast, Philipp Leonhard *(Karlsruhe Institute of Technology, Germany)*
Römer, Ulrich Johannes *(Karlsruhe Institute of Technology, Germany)*
Zirkel, Marten *(Technische Universität Ilmenau, Germany)*
Zentner, Lena *(Technische Universität Ilmenau, Germany)*
Fidlin, Alexander *(Karlsruhe Institute of Technology, Germany)*

Bipedal walking robots have been rapidly developed in the recent years, since they are capable of locomotion in complex terrains. Their flexibility has to be provided by a controller, which is designed based on certain model assumptions with the intension of achieving simplicity and robustness. One popular concept is the hybrid zero dynamics (HZD) control. It allows for highly efficient gaits, since the natural dynamics of the controlled system can be utilized. The gait at a constant average speed (step length over step duration) is regarded as a periodic sequence of the alternating single (SSP) and double support (DSP) phases. The feedback controller synchronizes the actuated joints to their reference trajectories. In the case of a vanishing control error, the periodic gait can be described by the limit cycle of the remaining zero dynamics with fewer degrees of freedom, which allows efficient simulations.

As a research focus, we investigate walking on a viscoelastic compliant ground [1]. The planar robot model consists of five rigid segments (an upper body, two thighs and two shanks), which are connected by four actuated revolute joints with integrated electric motors. Point feet are modeled at the lower end of the shanks. Furthermore, both SSP and DSP are modeled as non-instantaneous dynamics. The transition between both continuous phases is modeled by two discontinuous events: the touchdown of the swing leg at the end of the SSP, and the lift-off of the rear stance leg at the end of the DSP. Due to the compliant ground, no inelastic impact is considered during the touchdown event. A numerical optimization process locates the periodic solution for the hybrid zero dynamics' limit cycle, while the objective function (the cost of transport) is minimized [2]. The resulting energy efficiency as well as the gait stability under the influence of the ground compliancy will be presented, and compared against results for hard ground.

Acknowledgements:

This work is financially supported by the German Research Foundation (DFG), grant FI 1761/4-1 | ZE 714/16-1.

References:

[1] J. Alves, N. Peixinho, M. T. da Silva, P. Flores and H. M. Lankarani (2015): A comparative study of the viscoelastic constitutive models for frictionless contact interfaces in solids, Mechanism and Machine Theory, vol 85, pp. 172-188.

[2] U. J. Römer, C. Kuhs, M. J. Krause and A. Fidlin (2016): Simultaneous optimization of gait and design parameters for bipedal robots. Proceedings of ICRA 2016, pp. 1374-1381.

Comparing reference conditions of floating frame of reference formulations expressed in absolute boundary coordinates

van Voorthuizen, Karlijn *(University of Twente, Netherlands, The)* 15:00
Abdul Rasheed, Mohammed Iqbal *(University of Twente, Netherlands, The)*
Schilder, Jurnan *(University of Twente, Netherlands, The)*
Rosic, Bojana *(University of Twente, Netherlands, The)*

Floating frame formulations for flexible multibody systems are often expressed in a mixed coordinate set involving both absolute floating frame coordinates and local generalized coordinates. However, if expressed in the mixed set, the kinematic constraints take the form of nonlinear equations. Therefore, Lagrange multipliers are required to formulate the constrained equations of motion. Alternatively, defining a floating frame formulation only in terms of absolute interface coordinates, strongly simplifies the kinematic constraints. To obtain such a formulation, one needs to include reference conditions which eliminate the redundancy between the mixed coordinates and the absolute interface coordinates. The reference conditions allow one to derive an unique transformation matrix between the absolute interface coordinates and the mixed coordinate set. If the floating frame formulation is not restricted to modal reduction sets which can only describe elastic deformations, the reference conditions must take the form of six position-level constraints which remove the rigid movement from the elastic displacement. Three well established reference conditions of this type (a) define the floating frame attached to an interface point, (b) define the floating frame as a weighted average of the movement of the interface points and (c) define the floating frame attached at a node located at the center of mass of the undeformed body. The reference condition chosen to define the floating frame formulation influences the accuracy of the simulation results and computational cost of the resulting formulation. However, the choice between the reference conditions is complicated by the absence of comparisons between the resulting formulations and the independent derivations of the formulations. Therefore, this work will show that transformation matrices of similar structure can be derived for the three described reference conditions, which allows for examination of the similarities and differences between the definitions. Furthermore, the obtained transformation matrices are used to assess the performance of the floating frame formulations.

An experimental study on rotor interaction of fixed tilted UAV rotors

Bernstein, David *(TU Dresden, Germany)* 15:20
Bieber, Jonas *(TU Dresden, Germany)*
Beitelschmidt, Michael *(TU Dresden, Germany)*

Unmanned aerial vehicles (UAV) with parallel rotors, often called multirotors, have become increasingly popular in recent years to perform free flight tasks such as photography and inspection. These UAV are underactuated, because they cannot independently generate forces and torques in all 3 spatial directions. However, in the field of Aerial Manipulation, higher precision requirements and the need to apply contact forces make the use of fully-actuated UAVs worth considering. Full actuation can be achieved either by at least six fixed tilted rotors or a smaller number of actively tilted rotors. Both concepts can lead to interactions of the flow fields of the rotors.

The flight control of a UAV requires sophisticated control strategies, especially in the case of contact or manipulation tasks. In any case, model-based feedforward control is necessary. This requires knowledge of the relationship between motor speeds and the related spatial rotor forces and torques. Here also the interactions different rotors come into play.

For underactuated UAVs, the interaction between parallel rotors depending on their spacing is subject of numerous publications. To quantify the influence, especially rotor thrust, CFD simulations and experimental studies have been carried out. Comparing different publications, the influence calculated by CFD simulations is clearly overestimated compared to the experimental results. A relevant influence on the mean rotor thrust is not measured.

The Chair of Dynamics and Mechanism Design of TU Dresden has developed a fully actuated hexarotor with fixed tilted rotors for Aerial Manipulation. Pairwise, the rotors are closely spaced and tilted toward each other by about , resulting in intersecting thrust vectors and therefore interacting downstreams.

However, since the downstream interactions are much stronger in the fully actuated UAV configurations than in parallel rotors, the results of previous research cannot necessarily be transferred. In this paper, several experimental setups are presented. To investigate the influence of the rotor interaction on the spatial rotor forces and torques, the thrust motor is mounted in different directions at the top of uniaxial force or torque sensors. The influencing thrust motor is mounted decoupled from the other. No relevant changes in the mean forces and torques are measured even at high influencing rotor speeds. The force and torque fluctuations depending on the excitation order are also analyzed. Here, no clear correlation can be observed between high influencing rotor speeds and high rotor force and torque fluctuations.

Computationally Efficient Implementation of the Gauss-Newton Method for solving the Forward Kinematics of Redundant Cable-Driven Parallel Robots

Bieber, Jonas *(Technische Universität Dresden, Germany)* 15:40
Pallmer, Steffen *(Technische Universität Dresden, Germany)*
Beitelschmidt, Michael *(Technische Universität Dresden, Germany)*

Cable-driven parallel robots (CDPRs) are parallel robots in which cables are used instead of rigid connecting elements. An important task here, as in other areas of robotics, are kinematic

calculations. The state of the CDPR can be described either in Cartesian workspace coordinates as a pose or in the joint space via the cable lengths. The calculation of the cable lengths from a given platform pose is relatively simple for CDPRs. In contrast, the forward kinematics, i.e. the calculation of the pose from the cable lengths, is complex due to the parallel topology and often cannot be solved analytically. In addition CDPR systems are often designed redundantly, with more cables than Cartesian degrees of freedom. This redundancy causes that the solution of the forward kinematics can be considered as a fitting problem, where for measured cable lengths the solution with minimum error norm is sought. Common approaches to solve the forward kinematics are iterative approximation methods, such as the Gauss-Newton method. Here, the solution is approached stepwise starting from an initial starting pose. The pose estimation can be updated in each step using the Jacobian matrix of the inverse kinematics and the difference between measured and calculated cable lengths as solution of a linear system of equations. While the method is straightforward for translational coordinates, rotational coordinates require careful considerations. In this publication unit quaternions shall be used for describing the orientation. The advantage is that this representation is singularity-free, and allows computationally efficient calculations. However, these advantages over descriptions like Euler angles are at the cost of an additional fourth parameter. For the iterative solution procedure of forward kinematics, this results in the constraint of normalized unit quaternions. This publication proposes that the orientation should not be seen as a sum of stepwise orientation changes but as a continuous application of quaternion multiplication.This way the inclusion of the constraint in the system of equations to be solved can be avoided. Also, square-rooting to form the magnitude and normalize the quaternion is not required. This allows a computationally efficient implementation of the Gauss-Newton method for calculating the forward kinematics of CDPRs and possibly also other problems in the field of multibody dynamics.

S01-02: Multi-body dynamics

Date: June 1, 2023 16:00-19:00
Room: POT/351

Simplified Description of Hard Particles in Tribological Systems Using Statistical Sample Particles

Bilz, Raphael *(Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany)* 16:00
de Payrebrune, Kristin *(Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany)*

Technical applications often include tribological systems in which friction and wear occur. Hard particles such as sand are often present between the surfaces of the first bodies, affecting both the system dynamics and the resulting surface topography of the first bodies. Real tribological systems can contain a very high number of particles. Hence, for performance reasons, the explicit representation of each particle in a simulation model is often not practical.

The model presented here is based on a simplification by grouping several particles into statistical sample particles. This grouping into so-called “statistical sample particles” simplifies the motions of the individual particles, but the contact stiffness and orientation dependence of the force are still determined by the set of individual particles represented in the statistical sample, especially for small sample sizes.

Using sample size 1, each individual particle is represented without simplification, while using a sample size equal to the number of particles in the system, all particles in the system are combined to form a single statistical sample particle.

This approach provides a very simple way to specify the model complexity and desired level of detail for the particle representation within a model of a tribological system.

A soft Robot Gripper with Integrated Shape and Gripping-Force Sensors

Grube, Malte *(Hamburg University of Technology, Germany)* 16:20
Seifried, Robert *(Hamburg University of Technology, Germany)*

Soft material robots are an emerging and fast-growing field of research with potential applications in various fields. The modelling of soft robots requires often advanced methods from flexible multibody dynamics. The use of soft robots is particularly popular for gripping applications. Rigid grippers usually require complex control and are often only able to grip objects of a certain shape, which limits their applicability in real-world applications. In contrast, basic soft grippers often require no or very simple control and can often grip objects of very different shapes. Due to their soft structure, they can adapt to the shape of the gripped objects. Therefore, the control of soft grippers is still an open topic. For more complex gripping tasks, however, more advanced grippers are needed that require sensor feedback and control: For sensitive objects, it is important not to exceed the permissible gripping force in order to avoid damaging the object. This is usually best achieved with an enclosing grip. For other objects, however, a fingertip grip is more suitable. Therefore, the application range of soft grippers can be extended by integrating sensors into the gripper. The sensors make it possible to monitor and control the gripping process in order to achieve a uniform and

sufficiently secure grip. In this contribution the sensor integration and control for different gripping strategies of a three-finger gripper is presented. Both grip force sensors and shape sensors based on [1] are used for this purpose.

[1] M. Grube and R. Seifried, "An optical curvature sensor for soft robots," in ROMANSY 24 - Robot Design, Dynamics and Control, A. Kecskeméthy and V. Parenti-Castelli, Eds. Cham: Springer International Publishing, 2022, pp. 125-132.

Towards Intelligent Trajectory Planning of Air-to-Ground Coordinated Robot Motion

Chen, Jingshan *(Institute of Engineering and Computational Mechanics, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany)*
Ebel, Henrik *(Institute of Engineering and Computational Mechanics, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany)*
Luo, Wei *(Institute of Engineering and Computational Mechanics, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany)*
Eberhard, Peter *(Institute of Engineering and Computational Mechanics, University of Stuttgart, Pfaffenwaldring 9, 70569 Stuttgart, Germany)*

16:40

Whether in industry or daily life, the demand for scenarios where robots cooperate to transport objects increases. Ground-based robots can efficiently transport in well-accessible terrain over shorter distances, whereas air-based robots have advantages for express transports over rugged terrain. The combination of both can accommodate many transport requirements and topographic conditions. However, the limited flight duration of unmanned aerial vehicles (UAVs), especially with the added weight of the transported parcel, makes minimal transport time an essential consideration when planning trajectories. In this context, this contribution studies a scenario where an UAV picks up a transported object from a moving ground mobile robot.

In the existing literature on trajectory planning for cooperative transportation among robots, the point of object handover is manually determined a priori, and usually also some path waypoints are given. A priori fixed waypoints, however, will often yield a suboptimal solution, leading to a longer, less efficient transportation. Hence, this contribution proposes a method to autonomously determine the handover location and plan jointly an admissible trajectory for both ground mobile robot and UAV. We utilize the discrete mechanics and complementarity constraints (DMCC) method to determine the handover location with minimum mission time autonomously. This method enables simultaneously generating trajectories for both the UAV and the ground mobile robot by using complementarity constraints while considering the dynamics of all systems at the same time.

Currently, this method of planning has calculation times that are not real-time capable. Hence, we aim to make the planning process more efficient by learning an efficient surrogate model for the path planner using data-based methods. Moreover, while a well-planned path is important for a successful transportation, insight from hardware experiments shows that also the hardware design of the object-grabbing manipulator installed on the UAV has a substantial influence on the performance and the success of the transportation. Therefore, future work will look at the manipulator's design based on the generated optimal trajectory.

Stability investigations for Lie group integrators applied to dissipative systems

Arnold, Martin *(Martin Luther University Halle-Wittenberg, Germany)*
Tumiotto, Denise *(Martin Luther University Halle-Wittenberg, Germany)*
17:00

For increasing time, any two solution trajectories of a dissipative system will approach each other (in a suitable norm). In linear configuration spaces, this solution behaviour is characterized by one-sided Lipschitz conditions and by criteria for the logarithmic matrix norm or for the real parts of the Jacobian of the right hand side. There is a well developed theory to characterize the behaviour of time integration methods for dissipative systems in an equivalent way by A-, B- or G-stability and B-convergence. Kunzinger et al. (2006) have developed a framework for measuring distances between solution curves in nonlinear configuration spaces (M. Kunzinger, H. Schichl, R. Steinbauer, J. A. Vickers: *Global Gronwall estimates for integral curves on Riemannian manifolds*. - Rev. Mat. Comput., 19:133-137, 2006). For dissipative systems, the more recent work of Simpson-Porco and Bullo (2014) provides criteria for studying contractivity of analytical solutions in this setting (J.W. Simpson-Porco, F. Bullo. *Contraction theory on Riemannian manifolds*. - Systems & Control Letters, 65:74-80, 2014). Up to now, there is no equivalent theory for the time discretization of dissipative or contractive systems in nonlinear configuration spaces. In the present paper, we consider the application of implicit Lie group integrators to dissipative systems. The focus is on Lie groups that are isomorphic to Cartesian products of (multiples of) R^3, SO(3) and SE(3) and have been used successfully in the efficient dynamical simulation of flexible multibody systems with large rotations. For simple test problems like the planar rotation of a rigid body with a stiff torsional spring, the local parametrization based approach of Munthe-Kaas is shown to result in Lie group integrators that share one-to-one the known contractivity properties of their classical counterparts for systems in linear spaces. Situation gets substantially more complicated for more complex simulation scenarios. Therefore, simple low dimensional test problems like Dahlquist's test equation in linear spaces do not seem to be appropriate for characterizing the stability behaviour of Lie group integrators. The stability behaviour of implicit Lie group integrators that avoid the use of local parametrizations is even more complex and may suffer from an inherent explicit part of the discretization. These theoretical investigations will be illustrated by a comprehensive set of numerical results for test problems of increasing complexity. Acknowledgement: The authors acknowledge gratefully joint work on this topic with Elena Celledoni, Ergys Çokaj and Brynjulf Owren (NTNU Trondheim) in the Marie Skłodowska-Curie European Training Network THREAD (`https://thread-etn.eu/`).

Yarn modelling in textile machines using MBS, the reef-knot as example

Beitelschmidt, Michael *(TU Dresden, Germany)*
Krentzien, Maximilian *(TU Dresden, Germany)*
17:20

The dynamics of textile machines in one area of application of multi-body simulation (MBS). Until now the modelling of the threads and their dynamics had to be done with other modelling methods. In a new approach the yarn is implemented as transported, discrete beam based on the finite difference method in the MBS environment. The beams must on the one

hand represent the tension forces in the machine and on the other hand be able to form stitches and knots.

As example the forming of a reef-knot is shown. The model topology consists of two flexible bodies representing the yarns. Constraints are used to guide yarn specific starting and end node and joints with driven states are used to model the process of tying together two yarns. A contact force element between the yarn surfaces is implemented to map the process of knotting.

Additionally, an automatic initial geometry generation is part of the tool chain in order to investigate process influencing aspects such as bending stiffness and degree of discretisation. In general, the model is utilised to investigate the dynamical behaviour of the yarn in the context of MBS.

Furthermore, the research can be used to investigate the minimal curvature radius of a yarn in order to know to which extend a knot could reach its minimal tied size depending on the input parameters.

Fast determination of the points of contact for non-spherical particles and application to ellipsoids

Rebel, Ricardo *(Institut für Strömungsmechanik, Technische Universität Dresden, George-Bähr-Straße 3c, 01062 Dresden, Germany)*
Fröhlich, Jochen *(Institut für Strömungsmechanik, Technische Universität Dresden, George-Bähr-Straße 3c, 01062 Dresden, Germany)*

17:40

The transport of particles in fluid flow plays an extensive role in both industrial and environmental processes. Spatially resolved simulations of particle-laden flows, considering the interactions between the particles and the fluid as well as among the particles themselves, allow a better insight into the underlying physics of those processes. In such simulations, the inter-particle forces are calculated by using collision models that rely on the knowledge of the points of contact, which are analytically given in the case of spheres. Indeed, in practical applications, the particles are mostly modeled as being spherical. However, the particle shape may impact on the overall motion. It is therefore of interest to study flows containing a large number of non-spherical particles. Unlike their spherical counterpart, non-spherical particles require iterative procedures to approximate the point of contact up to a desired accuracy. Such methods can be derived from various concepts, leading to either optimization or root-finding problems for the minimum distance between the particles. Although several methods of this kind have already been proposed, many of them lack uniqueness of the solution, accuracy or computational efficiency. However, as the volume fraction of particles in the flow increases, so does the number of collisions, making them eventually dominate the motion. Hence, in order to perform simulations involving a large number of non-spherical particles in a reasonable amount of time, it is necessary to use efficient algorithms to solve the minimum distance problem. This contribution compares several promising methods in the context of ellipsoidal particles. Building upon these results, a combination of different existing approaches yields a nonlinear optimization problem that is treated with a globally convergent algorithm ensuring a unique solution in reasonable time. It is then shown that

this method is superior to a well-established algorithm for distance calculations in terms of computation time.

Linearization and change of observer for rotating discrete tire structures

Ruhwedel, Tobias *(Fraunhofer Institute for Industrial Mathematics, Germany)* 18:00

Especially with electrification of automobile industry and the construction of completely new chassis, the vibrational analysis of full vehicle systems remains an important field in vehicle development. The tire, as the interface between vehicle and road is an integral part of these systems. Linearization is an important tool when investigating and adapting the frequency response of such high dimensional systems. For a simple discrete, non-linear tire model we use its rotational symmetries to analyze the structure of the eigenspaces obtained by linearizing around a stable periodic orbit. We define a time-dependent change of coordinates that implements a change to a spatially fixed observer without explicitly assuming any underlying continuous material formulation. Finally, we investigate how Koopman eigenvalues and -functions of both systems are related to understand the change of observable vibrational behavior associated to such a coordinate transformation.

Towards a remote-access testbed for teaching mobile underwater robotics

Bauschmann, Nathalie *(Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TUHH), Germany)*
Duecker, Daniel A. *(Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TUHH), Germany; MIRMI - Munich Institute of Robotics and Machine Intelligence, Technical University of Munich (TUM), Germany)*
Seifried, Robert *(Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TUHH), Germany)* 18:20

Teaching students not just theoretical content but also exposing them to hands-on experience with physical systems is a crucial goal of modern engineering study programs. At the same time, autonomous mobile robotics is a wide and fast-growing research field. One interesting type of such mobile autonomous robotic systems are underwater robots which have various relevant applications, such as deep-sea exploration, environmental monitoring, and maintenance of underwater structures. With this, there is also growing demand for engineering students with experience in mobile autonomous robotics and particularly in the underwater domain.

While relevant topics in mobile robotics, such as mechanics, multibody dynamics, control theory, simulation, and machine learning are covered in different mechanical engineering, mechatronics, or computer science courses, there is often a clear lack of practical experience with real hardware. To address this gap, laboratory internships are often offered to provide practical connection to the course material. However, due to limited resources, these internships are usually aimed at teaching specific, narrowly defined content. Self-developed, open questions as well as critical questioning of the procedure are often neglected in this context. Overall, there is a need for hands-on learning opportunities that allow students to apply their knowledge in practical ways, while also fostering critical thinking, problem-solving, and teamwork skills.

We present “Roboquarium”, an interdisciplinary and remotely-accessible underwater robotics teaching/learning space that enables hands-on experience in combining machine and software development. Being able to access this experimental space from home or in hybrid teams maximizes possible lab time for students.

In terms of hardware, the Roboquarium consists of a 4 m x 2 m x 1.5 m water tank testbed, equipped with an underwater high-speed motion capture system. Besides providing a ground truth for evaluation of developed modeling and control strategies, this system is also used for safety features such as geofencing. Two BlueROV2 underwater robots with an adaptable sensor suite can be deployed in this testbed. Moreover, a 5 DOF arm with a gripper can be mounted to the robot. This especially allows the teaching of multibody dynamics related topics, such as modeling, simulation, parameter estimation and model-based control. In order to enable remote-access, cameras above and underwater are used. Remote robot control is achieved via VPN. Such a maritime remote-enabled experimental space is to the best of the authors’ knowledge so far unique around the world.

S02: Biomechanics

Organizer(s): **Röhrle, Oliver** *(U Stuttgart)*
Klinge, Sandra *(TU Berlin)*

S02-01: Biomechanics

Date: May 30, 2023 13:30-16:10
Room: POT/351

A New Approach for Analysing Motion and Deformation of Left Ventricle: Post-processing 3D Echocardiography Data with Finite Element Method

Cansiz, Baris *(Institute for Structural Analysis, TU Dresden)* 13:30
Sveric, Krunoslav *(Herzzentrum Dresden, TU Dresden)*
Linke, Axel *(Herzzentrum Dresden, TU Dresden)*
Kaliske, Michael *(Institute for Structural Analysis, TU Dresden)*

Stroke volume, ejection fraction, mass and size of the left ventricle (LV) are very important markers that are used by cardiologists in order to assess the global function and disease severity. Moreover, cardiologists often need to measure displacements, velocities, rotation, twist, torsion, strain and strain rates for a deeper investigation of the LV function. To this end, data obtained from 2D/3D echocardiography (echo) devices are analysed by a dedicated software. In the medical community, it is common practice to examine segmental (regional) values. For example, 3D echo data are analysed by dividing the LV endocardial surface into 16 or 17 areas (segments), which consist of several nodes (vortices) and the nodal values are averaged over the segments. Although, the averaged segment values provide useful information and are widely used, looking at pointwise values might enable a more extensive LV assessment, which has not been attracted attention so far. For instance, averaging might be ruling out unusual localized deformations, particularly in pathological cases, which can be only detected through a point-wise distribution. In this study, we aim to analyse LV motion and deformation from engineering perspective. We first export the tracked endocardial surfaces from 3D echo data by using the software 4D LV-Analysis from Tomtec Imaging Systems GmbH. The software discretizes the tracked surface over 862 nodes with 1720 triangular elements and enables to export the current coordinates of the nodes from the beginning of the systole to the ending of the diastole. Namely, the deformation state of LV endocardial surface is available at each time frame. From a computational perspective, the exported data is equivalent to obtaining the finite element solution of contracting LV. Once having the deformation state of the LV at hand, one can calculate any deformation related quantity in a pointwise manner such as displacement along preferred directions, strains, rotation and surface curvature. Furthermore, we will compare averaged segmental values to point-wise values over LV surface and discuss whether the point-wise values provide more information about local LV deformation than the averaged segmental values.

Combined Modeling of major mechanical aspects in arterial walls including active response, growth-based residual stresses and fiber reorientation

Uhlmann, Klemens *(Ruhr-Universität Bochum, Germany)* 13:50
Balzani, Daniel *(Ruhr-Universität Bochum, Germany)*

To investigate the risk of plaque rupture in atherosclerotic arteries and, hence, improve clinical practice with respect to medical treatments of cardiovascular diseases, computational simulations of arterial walls in health and disease are considered promising. Then, an accurate, mechanical description of various aspects of the arterial tissue is necessary to obtain realistic distributions of mechanical fields from numerical simulations. Next to the strongly nonlinear and anisotropic passive behavior of the wall, the contraction of smooth muscle cells (SMCs), a realistic fiber orientation as well as reasonable distributions of residual stresses have to be considered.

We propose a chemo-mechanical model which covers the mentioned, mechanical aspects of the arterial wall. The proposed mechanical model is designed to describe two different stretch-dependent mechanisms: a calcium-dependent and a calcium-independent contraction [1]. This design enables the description of the experimentally observed contraction of arteries as a reaction to increased internal pressure, which can be considered a crucial aspect of the regulatory mechanism of muscular arteries. Furthermore, the approximation of realistic fiber orientations and residual stresses is based on mechanically founded assumptions on the underlying adaptation processes, which are assumed to be stress-driven [2]. For the residual stresses, anisotropic growth is modeled by a multiplicative decomposition of the deformation gradient, where the growth tensor itself is decomposed into three parts associated to the directions of the principal stresses. An algorithmic framework for the implementation of all mechanical aspects of the arterial model in finite element programs will be presented. Based thereon, simulation results of arterial rings under intravascular pressure will be analyzed. The quality of resulting mechanical fields, i.e., stresses and stretches, will demonstrate that no realistic results can be expected from simulations where not all relevant mechanical aspects are considered.

[1] K. Uhlmann and D. Balzani. Chemo-Mechanical Modeling of Smooth Muscle Cell Activation for the Simulation of Arterial Walls under Changing Blood Pressure. Biomech. Model. Mechanobiol., in press.

[2] A. Zahn and D. Balzani. A combined growth and remodeling framework for the approximation of residual stresses in arterial walls. Z. Angew. Math. Mech., 98:2072 2100, 2018.

Comparative Computational Studies of Left Ventricular Strains using Hyperelastic Active Frameworks

Ogiermann, Dennis *(Department of Civil and Environmental Engineering, Ruhr University Bochum, Universitätsstraße 150, 44801 Bochum)*
Perotti, Luigi E. *(Mechanical and Aerospace Engineering, University of Central Florida, 12760 Pegasus Drive, Orlando, FL, 32816)*
Balzani, Daniel *(Department of Civil and Environmental Engineering, Ruhr University Bochum, Universitätsstraße 150, 44801 Bochum)*

14:10

Mathematical models of the human heart are critical to improve our fundamental understanding of cardiac function and therefore the treatment of patients with cardiac diseases. Over the last two decades, three major frameworks for the active response of cardiac tissue have emerged: the active stress, active strain, and generalized Hill framework. Two of the most common validation strategies consist of reproducing selected experimental responses at the tissue level and/or pressure-volume loops at the ventricular level. It has been shown that all frameworks can meet reasonably well these validation criteria. However, studying the analytical properties of these frameworks reveals that their response may differ even in very simple cases. This raises the question of which additional validation criteria should be considered and which key differences across frameworks they can highlight.We will first present an analysis of these frameworks formulated using classical invariants to highlight advantages and limitations of each approach as used in literature. Based on this analysis, we will propose an extended version of the generalized Hill framework. The equibiaxial experiments of Lin and Yin (1998) testing active cardiac tissue are used to validate the material point response. Cardiac strain measurements are then utilized to validate the structural response in an idealized left ventricular model. It is shown that these two criteria can differentiate the model responses and provide critical insights into the accuracy of each approach. Here, our extended formulation of the generalized Hill framework with an active deformation gradient based on mesoscale rearrangement is shown to describe the response of cardiac tissue more accurately than commonly utilized models, while also providing a connection to physiological mechanisms.

Coupling of a poroelastic model to a vascular tree with application in liver modeling

Ebrahem, Adnan *(TU Darmstadt, Germany)*
Gangwar, Tarun *(TU Darmstadt, Germany)*
Jessen, Etienne *(TU Darmstadt, Germany)*
ten Eikelder, Marco F.P. *(TU Darmstadt, Germany)*
Mika, Michał Łukasz *(TU Darmstadt, Germany)*
Schillinger, Dominik *(TU Darmstadt, Germany)*

14:30

Over the last few decades, the theory of porous medium has been subject of many theoretical and numerical studies due to its potential applications in a variety of engineering fields ranging from civil, chemical and geotechnical engineering to biological, medical and material sciences [1].

In biomechanics, hard and soft tissues can be considered as deformable, permeable and porous media. This work is motivated by modeling blood flow through the vascularized human liver. In previous studies of the liver, either perfusion models [2] or tissue deformation [3] have been considered. However, since the liver is characterized by a high degree of vascularization, blood perfusion and tissue deformation are closely linked. Investigating the influence of perfusion on the steady-state mechanical behavior of the liver is of utmost importance due to possible application in surgical planning and surgery assessment. A detailed understanding of liver mechanics in relation to perfusion significantly improves many clinical treatment strategies, including suitable cut patterns during liver resections.

In order to achieve the coupling, we propose a two-phase poroelastic model coupled with a fluid network to describe tissue deformation and blood flow. In this contribution, we derive a set of equations for finite strain poroelasticity with application to the entire liver coupled to a vessel tree. We present numerical examples, demonstrating the capability of the methodology to model the poroelastic behavior of the liver.

[1] Ehlers, W., Bluhm, J., 2002. Porous media: theory, experiments and numerical applications. Springer Berlin, Heidelberg.
[2] Rohan, E., Lukeš, V., Jonášová, A., 2018. Modeling of the contrast-enhanced perfusion test in liver based on the multi-compartment flow in porous media. J. Math. Biol. 77.2, 421-454.
[3] Zheng, Y., Jiang, Y., Cao, Y., 2021. A porohyperviscoelastic model for the shear wave elastography of the liver. J. Mech. Phys. Solids 150, 104339.

Using Anisotropic Voronoi Tessellations to connect Arterial and Venous Synthetic Hepatic Trees

Jessen, Etienne *(Institute of Mechanics, Computational Mechanics Group, Technical University of Darmstadt, Germany)*
Steinbach, Marc C. *(Institute of Applied Mathematics, Leibniz University Hannover, Germany)*
Debbaut, Charlotte *(IBiTech-BioMMeda, Ghent University, Belgium)*
Schillinger, Dominik *(Institute of Mechanics, Computational Mechanics Group, Technical University of Darmstadt, Germany)*

14:50

Functional assessment of the liver is essential for increasing the success of treatment strategies, such as hepatic resection. However, the obtainable vascular data *in vivo* is limited by the maximum resolution of current imaging technologies. Synthetic generation of vascular trees *in silico* can potentially fill in the missing data to recreate the complete vasculature.

We extend our current synthetic generation method [1] to allow the coupled generation of multiple non-intersecting vascular trees up to the microcirculation. We utilize Voronoi tessellations to partition the space between the vascular trees. By inserting an appropriate Riemann metric [2], the resulting anisotropic Voronoi cells mimic the geometric structure of hepatic lobules, the functional units of the liver.

We test our new framework against a detailed corrosion cast of a human liver [3]. Our synthetic vasculature can closely follow the available physiological corrosion cast data across all scales.

References

[1] Jessen, E., Steinbach, M. C., Debbaut, C., & Schillinger, D. (2022). Rigorous mathematical optimization of synthetic hepatic vascular trees. *J R Soc Interface*, *19*(191), 20220087.
[2] Du, Q., & Wang, D. (2005). Anisotropic centroidal Voronoi tessellations and their applications. *SISC*, *26*(3), 737-761.
[3] Debbaut, C., Segers, P., Cornillie, P., Casteleyn, C., Dierick, M., Laleman, W., & Monbaliu, D. (2014). Analyzing the human liver vascular architecture by combining vascular corrosion casting and micro-CT scanning: a feasibility study. *J. Anat.*, *224*(4), 509-517

Switchless constitutive relation for passive myocardium that accounts for the distinct load-bearing characteristics of collagen and muscle fibers in compression

Tammisetti, Hari Sai Chaitanya *(Indian Institute of Technology Madras, India)*
K, Arvind *(Indian Institute of Technology Madras, India)*
Kannan, Krishna *(Indian Institute of Technology Madras, India)*

15:10

Unlike collagen fibers which cannot sustain compressive loads, muscle fibers in cardiac tissue may sustain some level of compression owing to their larger diameter and also due to their crosslinks with the collagen fibers. On using a novel matched-invariant whose value during compression: 1) is exactly zero for the collagen fibers and 2) ranges between zero and a maximum for the muscle fibers, determined by the level of crosslinking, the compressive load-bearing hypothesis is achieved in the orthotropic hyperelastic modeling of passive myocardium. Therefore, a tension-compression switch criterion is not required. The dispersion of the fibers is taken into account using the framework developed by Gasser, Ogden, and Holzapfel using the Generalized Structure Tensor approach, allowing for the direct incorporation of microstructural information into the constitutive relation. It is demonstrated that the model predictions coincide quite well with the biaxial and triaxial shear responses reported in the literature. As an added advantage, the matched-invariant naturally involves the I5 invariant, eliminating the constitutive defect of identical shear responses that results from modeling soft tissues using only the I4 invariant.

S02-02: Biomechanics

Date: May 31, 2023 08:30-09:30
Room: POT/351

A novel modeling approach for stress-driven anisotropic growth of bioengineered tissues

Brepols, Tim *(RWTH Aachen University, Germany)* 08:30
Holthusen, Hagen *(RWTH Aachen University, Germany)*
Rothkranz, Christiane *(RWTH Aachen University, Germany)*
Lamm, Lukas *(RWTH Aachen University, Germany)*
Reese, Stefanie *(RWTH Aachen University, Germany)*

The field of medical research utilizing bioengineered tissues, such as in the case of biohybrid heart valves, has seen a significant increase in recent years. This has led to a growing need for efficient computational models to be used in biomechanical applications. In response to this, various approaches have been developed that consider the processes of finite growth and remodeling in bioengineered tissues. All these advancements aim to tackle contemporary medical issues and enhance patient care. The present study intends to make another valuable contribution to the above-mentioned topic and to gain further insights. For this, a recently developed material model is presented and discussed (see [1]) which takes into account the remodeling of tissue and the orientation of collagen fibers. It is based on the well-established multiplicative decomposition of the deformation gradient into elastic and growth-remodeling parts (see [2]), and makes use of a structural tensor to represent the fiber direction. Furthermore, the evolution equations for growth and remodeling are derived from homeostatic surfaces serving as inelastic potentials (see [3]) and the remodeling of collagen fibers towards the principal stress is realized similarly to, for example, [4]. As shown in [1], the formulation makes use of a novel co-rotated intermediate configuration concept, which greatly facilitates, e.g., the application of automatic differentiation during the model's implementation. Finally, the good behavior of the model as well as its flexibility in application are demonstrated in structural simulations and the results are qualitatively compared to experimental data from the literature.

[1] H. Holthusen, C. Rothkranz, L. Lamm, T. Brepols, and S. Reese, Journal of the Mechanics and Physics of Solids 172, 105174 (2023).
[2] E. Rodriguez, A. Hoger, and A. McCulloch, Journal of Biomechanics 27, 455 - 467 (1994).
[3] L. Lamm, H. Holthusen, T. Brepols, S. Jockenhövel, and S. Reese, Biomechanics and Modeling in Mechanobiology 21, 627-645 (2022).
[4] E. Kuhl, K. Garikipati, E. Arruda, and K. Grosh, Journal of the Mechanics and Physics of Solids 53, 1552-1573 (2005).

Characterisation of the layer, direction and time-dependent mechanical behaviour of the human oesophagus and the effects of formalin preservation

Hossain, Mokarram *(Swansea University, United Kingdom)* 08:50
Durcan, Ciara *(Swansea University, United Kingdom; University of Grenoble Alps)*
Chagnon, Gregory *(University of Grenoble Alps)*
Peric, Djordje *(Swansea University, United Kingdom)*
Girard, Edouard *(University of Grenoble Alps)*

The mechanical characterisation of the oesophagus is essential for the applications of medical device designs, surgical simulations, tissue engineering and for the investigation of the organ's pathophysiology. However, the material behaviour of the oesophagus has not been fully established using fresh human tissue, particularly in regard to the organ's layer-dependent response. As of yet, in literature, only the hyperelastic response of the intact wall has been studied. Therefore, in this study, the layer-dependent, anisotropic, visco-hyperelastic behaviour of the human oesophagus was investigated through various mechanical tests. For this, cyclic tests with increasing stretch levels were carried out in both the longitudinal and circumferential directions of each oesophageal layer at two different strain rates. Additionally, stress-relaxation tests of the different oesophageal layers were conducted in both directions. To assess the residuals strains of the organ, zero-stress state analysis was carried out via the opening angle method. Overall, the results show discrete properties in each layer and direction, highlighting the importance of treating the oesophagus as a multi-layered composite material.

A comparison between the fresh and embalmed tissue behaviour was carried out and surprisingly revealed similarities in terms of anisotropy, strain-rate dependency, stress-softening and hysteresis, with the main difference between the two preservation techniques being the magnitude of these properties. As formalin fixation is known to notably affect the formation of cross-links between the collagen of biological materials, the similarities may reveal the influence of cross-links on the mechanical behaviour of soft tissues.

Exploring the reason for tension and compression stress-strain asymmetry observed in passive skeletal muscle

Mohammadkhah, Melika *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany)* 09:10
Murphy, Paula *(Department of Zoology, School of Natural Science, Trinity College Dublin, Ireland)*
Klinge, Sandra *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany)*
Simms, Ciaran *(Trinity Centre for Bioengineering, Department of Mechanical and Manufacturing Engineering, Trinity College Dublin, Ireland)*

For many years, only the force producing capabilities of skeletal muscle was of interest. However, the mechanics of passive skeletal muscle are important in many biomechanical applications such as impact biomechanics and rehabilitation engineering. An adequate explanation for the tension/compression asymmetry observed in the stress-strain response of skeletal muscle and the role of Extra Cellular Matrix (ECM) as a contributor to stress response remains elusive. Therefore, the overall aim of this study is to advance the knowledge of the

passive mechanical behaviour of skeletal muscle, and its relation to the microstructure of the muscle through combined experimental, microstructural and computational approaches.

From the experimental point of view, mechanical testing of skeletal muscle of chicken and porcine tissue was conducted to observe the different stress-strain asymmetry between species. Since collagen in ECM is the main structural protein in connective tissues, it is believed to be primarily responsible for their passive load-bearing properties. The optimised protocol of visualisation of collagen was applied to report qualitatively and quantitatively on skeletal muscle ECM reorganization during applied deformation using a combination of CNA35 binding protein and confocal imaging of tensile and compressive deformation of porcine and chicken muscle samples applied in both the fibre and cross-fibre directions. Results show the overall three-dimensional structure of collagen in perimysium visible in planes perpendicular and parallel to the muscle fibres in both species. Furthermore, there is clear evidence of the reorganization of these structures under compression and tension applied in both the muscle fibre and cross-fibre directions, which generally explains anisotropy observed in the stress-strain response for both tissues. These observations improve our understanding of how perimysium responds to three-dimensional deformations. The three-dimensional illustration of perimysium structure was then used as a basis to create a microstructural-geometrical model to predict the passive mechanical stress-strain response observed in skeletal muscle. The current model represents the whole muscle response as a combination of both a group of muscle fibres (fascicle) response and the perimysium (ECM) response. It shows that although perimysium was believed to be a key element in the muscle stress response, the muscle fibres also contribute to stress-stretch response since the order of magnitude for the stress in muscle fibres is similar to that of perimysium. The model yields a good prediction of the whole muscle behaviour in Tension-Fibre and Compression-Fibre deformations using the optimum values for the model parameters obtained from the sensitivity studies.

S02-03: Biomechanics

Date: June 1, 2023 08:30-10:30
Room: POT/351

A unified approach for data- and continuum-mechanical-driven simulations of tumours in brain tissue

Suditsch, Marlon *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, University of Stuttgart, Germany)*
Ricken, Tim *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, University of Stuttgart, Germany)*
Wagner, Arndt *(Institute of Applied Mechanics, Chair of Continuum Mechanics, University of Stuttgart, Germany)*

08:30

A short remaining life expectancy and high mortality characterise brain tumours as a particularly dangerous disease. Simulations of the relevant processes of tumour growth and regression in brain tissue are realised by a continuum-mechanical model in the framework of the Theory of Porous Media (TPM), that is embedded in a data-integrated workflow. This workflow is based on suitable patient-specific data, that is basically available, e. g. from magnetic resonance images (MRI). Preparing the data by a set of tools, for example using a convolutional neural network in a shape of an U-Net, result in the segmented position and composition of the tumour and provide the referential geometry of an initial boundary value problem (IBVP). Furthermore, relevant information, e. g. about heterogenities or flow properties, are collected by image-processing tools. A numerically more efficient surrogate model based on the ratio of the composition of the tumour compartments is developed and calibrated with simulations of the TPM model. These modularly arranged components of the developed data-integrated approach are processed using the finite-element framework FEniCS and allow to study relevant clinical questions.

A Data-Driven Constitutive Model for Soft Biological Tissues

Açan, Alp Kağan *(Middle East Technical University, Turkiye)*
Tikenoğulları, Oğuz Ziya *(Middle East Technical University, Turkiye; Stanford University, United States of America)*
Dal, Hüsnü *(Middle East Technical University, Turkiye)*

09:10

Constitutive modeling of soft biological tissues is crucial for biomedical simulations and a deep understanding of tissue mechanics. Classical constitutive models have a fixed mathematical expression[1,2], however, the microstructure and the corresponding macro-mechanical response of different tissue types can vary significantly. A model that works for one tissue may not work for another kind of tissue, and choosing the right model may become challenging. To solve this issue, this study introduces a new data-driven approach to creating a unified model for predicting the mechanical response of various tissue classes. The proposed model is based on B-Spline approximations and assumes the strain energy function can be divided into volumetric, isotropic, and anisotropic components[3,4,5]. The B-Spline ansatz replaces partial derivatives with control points and polynomial degree, and allows the use of existing dispersion models[6]. The model adapts its control point values to reduce the error between data

and prediction until a threshold is reached, and is thermodynamically consistent through the use of optimization constraints[7]. The model is demonstrated on various biological tissues, showing excellent fitting capabilities with a minimal number of control points. The results of finite element simulations using this model are compared to the established Holzapfel-Ogden model[2]. The outcome is a generic framework that can model any tissue given the data from experiments and imaging techniques.

References

[1] Kuhl, E., Garikipati, K., Arruda, E. M., & Grosh, K. (2005). Remodeling of biological tissue: mechanically induced reorientation of a transversely isotropic chain network. Journal of the Mechanics and Physics of Solids, 53(7), 1552-1573.
[2] Holzapfel, G. A., & Ogden, R. W. (2009). Constitutive modelling of passive myocardium: a structurally based framework for material characterization. Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences, 367(1902), 3445-3475.
[3] Denli, F. A., Kaliske, M., Açan, A. K., Tüfekçioğlu, M. E., & Dal, H. (2022). Data driven constitutive modelling of rubberlike materials. In Constitutive Models for Rubber XII (pp. 105-111). CRC Press.
[4] Dal, H., Denli, F. A., Kaliske, M., & Açan, A. K. (2023). Data-driven constitutive modeling of rubberlike materials. Manuscript in preparation.
[5] Açan, A. K., Tikenoğulları, O. Z., Kuhl, E., & Dal, H. (2023). Data-driven modeling of anisotropic soft biological tissues. Manuscript in preparation.
[6] Holzapfel, G. A., Ogden, R. W., & Sherifova, S. (2019). On fibre dispersion modelling of soft biological tissues: a review. Proceedings of the Royal Society A, 475(2224), 20180736.
[7] Schröder, J., & Neff, P. (2003). Invariant formulation of hyperelastic transverse isotropy based on polyconvex free energy functions. International Journal of Solids and Structures, 40(2), 401-445.

Constitutive Artificial Neural Networks (CANNs) with applications to soft biological tissues

Linka, Kevin 09:30
Cyron, Christian J. *(Institute for Continuum and Material Mechanics, Hamburg University of technology, Germany; Institute of Material Systems Modeling, Helmholtz-Zentrum Hereon)*

The classical, theory-driven approach to describe the deformation of a material body relies on the formulation of constitutive equations relating strains and stresses. A drawback of this approach are the efforts typically required to develop appropriate functional relations and identify material parameters .These efforts are not required in data-driven approaches to constitutive modeling. To combine the advantages and overcome the disadvantages of both theory- and data-driven constitutive modeling, we have developed the novel concept of Constitutive Artificial Neural Networks (CANNs). This machine learning approach to data-driven constitutive modeling does not require any major a priori assumptions about the constitutive law but yet incorporates substantial theoretical knowledge about continuum mechanics and constitutive theory. This way, CANNs are able to learn the constitutive law of a material from

relatively small amounts of stress-strain data. Moreover, by their ability to incorporate also non-mechanical data, they cannot only describe the constitutive behavior of known materials but also predict the one of new materials, making them the ideal tool for computational biomechanics. Using data from mechanical tests, histological analyses and advanced imaging, this architecture is trained to predict the nonlinear macroscopic mechanical properties of e.g. arterial and brain tissue. Moreover, we demonstrate that our machine learning architecture is not limited to predictions but can also help to understand the mechanics of soft tissue. Using advanced concepts of explainable artificial intelligence, we demonstrate that it enables the automatic, systematic and largely unbiased quantification of the importance of different.

Deep learning-based surrogate modeling of coronary in-stent restenosis

Shi, Jianye *(Institute of Applied Mechanics, RWTH Aachen University, Germany)* 09:50
Manjunatha;, Kiran *(Institute of Applied Mechanics, RWTH Aachen University, Germany)*
Reese, Stefanie *(Institute of Applied Mechanics, RWTH Aachen University, Germany)*

Coronary artery disease (CAD) is one of the largest causes of death worldwide. Percutaneous coronary intervention (PCI) is one of the minimally invasive procedures used to overcome CAD by restoring blood flow in clogged coronary arteries. Unfortunately, PCI is associated with several risk factors including in-stent restenosis and stent thrombosis. Drug-eluting stents were developed to counteract the severe restenosis observed after bare-metal stent implantation. The risk of restenosis still prevailed due to the inhibitory effect of the drug on endothelial healing. The current work focuses on developing a multiphysics-based surrogate model using a deep learning framework to include the effect of anti-inflammatory drugs embedded in the drug-eluting stents. The highly resolved multiphysics model is based on a set of coupled partial differential equations (PDEs), which govern the mechanism of neointimal hyperplasia by capturing the effects of platelet aggregation, growth-factor release, cellular motility, endothelial barrier function and drug deposition.

Prescribed-motion and quasi-steady CFD of left ventricular hemodynamics – comparison to 4D flow MRI data

Obermeier, Lukas *(Institute of Computer-assisted Cardiovascular Medicine, Deutsches Herzzentrum der Charité, Berlin, Germany)*
Vellguth, Katharina *(Institute of Computer-assisted Cardiovascular Medicine, Deutsches Herzzentrum der Charité, Berlin, Germany)*
Wiegand, Moritz *(Institute of Computer-assisted Cardiovascular Medicine, Deutsches Herzzentrum der Charité, Berlin, Germany)*
Hellmeier, Florian *(Institute of Computer-assisted Cardiovascular Medicine, Deutsches Herzzentrum der Charité, Berlin, Germany)*
Goubergrits, Leonid *(Institute of Computer-assisted Cardiovascular Medicine, Deutsches Herzzentrum der Charité, Berlin, Germany; Einstein Center Digital Future, Berlin, Germany)*

10:10

Left ventricular (LV) hemodynamics are hypothesized to serve as indicator for the manifestation of cardiovascular diseases in early states. In the analysis of hemodynamics, computational fluid dynamics (CFD) can complement medical imaging methods for in-depth flow investigations. To potentially enable transfers into the clinic, verification, and validation of these CFD models is required. In this study, we compare the computed hemodynamics of two CFD approaches of different fidelity to 4D flow magnetic resonance imaging (MRI) data of three healthy subjects.

MRI data was acquired in a 1.5T MRI scanner. The LV geometrics were segmented from cine-short axis, end-diastolic whole heart, cine aortic valve (AV), and a rotational sequence for the mitral valve (MV). 4D flow data was acquired in a three-chamber view, as well as for the whole 3D LV cavity. The segmentations were used as boundary conditions (BCs) for the two CFD approaches developed earlier. In the first method (high fidelity), the LV motion is prescribed as BC in an Arbitrary-Lagrangian-Eulerian manner. The whole cardiac cycle is computed. The second approach (low fidelity) is based on a quasi-steady setup, where the ventricular volume change is modelled via a volume flux BC at the LV. Both approaches incorporate a 3D stiff MV modelled via porous media theory.

The flow rates derived from the geometric reconstructions as well as the 4D flow MRI data agree well. The CFD results show comparable flow patterns to 4D flow MRI data as visible from 3D streamlines, line probe velocities, and the vorticity a three-chamber view: a diastolic inflowing jet being accompanied by a ring vortex. The valve velocities take a likewise temporal course with relative errors at peak systole and peak E-wave below 15% in all cases. Towards late diastole, the flow field in the quasi-steady approach starts deviating from the prescribed-motion approach and the 4D flow MRI data. In terms of kinetic energy around E-wave, results take the same qualitative course, while MRI-based kinetic energy is slightly higher. In terms of computational expenses, the quasi-steady approach is computed 2-3 times faster.

Both CFD approaches deliver reasonable kinematics in comparison to 4D flow MRI. The quasi-steady approach delivers consistent results in early diastole, the prescribed-motion approach for the entire cardiac cycle with the downside of being computationally more expensive.

S02-04: Biomechanics

Date: June 2, 2023 08:30-10:30
Room: POT/351

Modeling the finite viscoelasticity of brain tissue based on microstructural information

Reiter, Nina *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)* 08:30
Paulsen, Friedrich *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
Budday, Silvia *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*

Continuum-mechanics-based computational models are a valuable tool to advance our understanding of mechanics-related physiological and pathological processes in the brain. Current numerical predictions of brain tissue behavior are mainly based on phenomenological material models. Such models rely on parameters that often lack physical interpretation and only provide adequate estimates for brain regions with a similar microstructure as those used for calibration. These issues can be overcome by establishing advanced constitutive models that are microstructurally motivated and account for regional and temporal changes through microstructural parameters.

To identify the microstructural mechanisms that underlie the tissue's macroscopic nonlinear and time-dependent mechanical response, we perform simultaneous compressive mechanical loadings and microstructural analyses of porcine brain samples. We propose a microstructure-informed finite viscoelastic constitutive model for brain tissue based on experimental insights into the link between macroscopic deformations and cell displacements. We use cellular displacement curves to determine a relaxation time constant and introduce hyperelastic model parameters as linear functions of the cell density. The model is calibrated using a combination of cyclic loadings and stress relaxation experiments in compression. The insights from this study provide a basis for the development of microstructure-based viscoelastic constitutive models for brain tissue, which may ultimately allow us to capture regional material heterogeneities and predict how tissue mechanics change during development, aging, and disease.

Multifield computational model for human brain development: explicit numerical stabilization

Zarzor, Mohammad Saeed *(FAU University, Germany)* 08:50
Steinmann, Paul *(FAU University, Germany)*
Budday, Silvia *(FAU University, Germany)*

The morphological surface of the human brain is still puzzling to scientists. During the last few decades, studies have addressed different aspects of this phenomenon. The underlying cellular processes occurring at the microscopic scale are certainly important for the folding process. However, there is also an essential contribution from mechanical forces generated at the macroscopic scale during these processes. Many previous studies confirmed this fact, but still, most of them have not considered the link between cellular processes and mechanical forces. Recently, we have explained how the proliferation in different zones of the brain, cell migration, and neuronal connectivity affect the folding through a multifield computational

model coupling an advection-diffusion model with the theory of finite growth. Besides the deformation, we introduce multiple fields representing the density of different brain cells, including radial glial cells, intermediate progenitor cells, outer radial gilia cells, and neurons, to study their effect on the resulting folding pattern. We mathematically describe the cellular behavior of each cell type to control mechanical growth in both radial and circumferential directions. To deal with issues regarding numerical stability of the advection-diffusion equation, which lead to temporal and spatial numerical oscillations, reduced efficiency of the numerical solver, and inaccurate results, we test different previously proposed stabilization methods. We highlight their individual strengths and weaknesses and adopt an artificial viscosity, which we apply only when the actual cell density does not satisfy the balance equation. The proposed method significantly improves the simulation results without additional numerical cost and allows us to study brain development in 2D and 3D. We finally show how the proposed model successfully mimics normal brain development.

Towards a multiscale framework for patient-specific liver simulation

Gerhäusser, Steffen *(Institute of Structural Mechanics and Dynamics, University of Stuttgart, Germany)*
Lambers, Lena *(Institute of Structural Mechanics and Dynamics, University of Stuttgart, Germany; Experimental Transplantation Surgery, Department of General, Visceral and Vascular Surgery, Jena University Hospital, Germany)*
Mandl, Luis *(Institute of Structural Mechanics and Dynamics, University of Stuttgart, Germany)*
König, Matthias *(Systems Medicine of the Liver Lab, Institute for Theoretical Biology, Humboldt-University Berlin, Germany)*
Ricken, Tim *(Institute of Structural Mechanics and Dynamics, University of Stuttgart, Germany)*
09:10

The liver performs vital functions in the human body, such as detoxifying drugs and synthesizing proteins, and is therefore essential for overall health. Liver diseases such as non-alcoholic fatty liver disease (NAFLD) or liver cancer represent a significant proportion of western lifestyle diseases. To combat these diseases, digital medicine in the field of simulation technology offers enormous potential for predictive treatment or surgical planning [1].

Here we present the development of a multiscale mathematical model based on the coupling of the tissue and cellular scales integrated with the whole-body scale. Within the Theory of Porous Media (TPM, see [2]), the hepatic lobule can be modeled as a multiphasic porous solid with advective and diffusive blood transport using multicomponent mixture theory. Partial differential equations (PDEs) describe the interplay between function, perfusion, and deformation, with the hepatic lobule discretized using the finite element method (FEM). At the lower scale, the metabolic processes in the cell can be modeled as biochemical reaction networks using ordinary differential equations (ODEs). The amounts of dissolved substances in the blood phase are communicated from the macroscale (tissue) to the microscale (cell), while the microsimulation provides sink/source terms for the balance equations of the macrosimulation. The microsimulation itself tracks intracellular substances and state variables that affect drug elimination and cell survival. The coupled model is benchmarked with a test compound metabolism as an example of liver function, where a substrate is enzymatically converted to a

product and possible toxic side products. The coupling is also characterized by the combination of domain-specific solvers, integrating a software library for high-performance simulation [3] of Systems Biology Markup Language (SBML) [4] based models into a framework for the FEM.

Furthermore, the multiscale liver model is coupled to an ODE-based physiologically based pharmacokinetics (PBPK) model at the whole-body scale, which includes the systemic circulation and organs relevant for drug detoxification besides the liver, such as the kidneys (e.g. [5]). In this setup, the whole-body model provides the boundary conditions for the FEM simulation, while the FEM simulation provides the boundary conditions for the ODE system.

The research also includes software specific aspects such as performance issues and introduces alternatives to the conventional coupling approach such as black box schemes. Finally, a comparison with alternative modeling approaches and experimental data is addressed, bringing the framework one step closer to an accurate decision support tool for everyday clinical use.

[1] Christ,B.,[...],König,M.,[...],Lambers,L.,[...]Ricken,T.,et al. Frontiers in Physiology(2021)12
[2] Ehlers,W. Foundations of multiphasic and porous materials(2002)
[3] Welsh C,[...], König M, et al. Bioinformatics. 2023(1)
[4] Keating SM,[...], König M, et al. Mol Syst Biol. 2020(8)
[5] Grzegorzewski J,[...], König M., et al. Front Pharmacol. 2022(13)

Vibration analyses of a mandible

Vulović, Aleksandra *(Faculty of Engineering, University of Kragujevac, Serbia; Bioengineering Research and Development Center (BioIRC), Serbia)*
Geroski, Tijana *(Faculty of Engineering, University of Kragujevac, Serbia; Bioengineering Research and Development Center (BioIRC), Serbia)*
Gogilan, Umaaran *(Ruhr-Universität Bochum, Germany)*
Saveljić, Igor *(Bioengineering Research and Development Center (BioIRC), Serbia; Institute for Information Technologies, University of Kragujevac, Serbia)*
Nestorović, Tamara *(Ruhr-Universität Bochum, Germany)*
Filipović, Nenad *(Faculty of Engineering, University of Kragujevac, Serbia; Bioengineering Research and Development Center (BioIRC), Serbia)*

09:30

Careful treatment of medical patients represents a primary requirement. Available expertise in the field contributes to the success of treatments, but striving and extending the knowledge enables significant improvements in the course of a patient's treatment. Our field of interest was focused on the influence of vibrations on the human body which may be related to patient treatment in postoperative, healing, or standard medical treatment phases. Particularly, the vibration behavior of the upper part of the human skeleton should be addressed, namely the skull and its parts. Understanding the vibration response of a human body may play an important role in some postoperative processes, during transportation, treatments, etc. Although some work on vibration analyses of a human skull has been recorded in the literature to the authors' best knowledge thorough, detailed, and systematic analyses of the vibration behavior of the mandible have not been performed yet. This was the motivation for this paper. We were focused on the investigation of the vibration behavior of a part of the human skull, namely a mandible.

In this work, we present an investigation of the relevant frequency range for the vibration analyses and the results that were obtained through these analyses that were covering the range of interests. Concerning the structural behavior, it is known that the excitations in a lower frequency range may be responsible for exciting dominant vibration modes. Yet, the behavior in higher frequency ranges may be of particular interest in cases where high-frequency resonance may be invoked. One example of this situation occurs in regular dental treatment due to interaction with rotating dental instruments. In this work, the frequency analyses of a mandible were performed using a 3D mandible model. The mandible model was developed through the segmentation of mandible CT scans and then manually refined for analysis. All parameters necessary for simulations were adapted from the literature.

In vitro study design derived from an in vivo lifting task

Brenzel, Katharina *(Institute for General Mechanics, RWTH Aachen University)* 09:50
Johnen, Laura *(Institute of Industrial Engineering and Ergonomics, RWTH Aachen University)*
Praster, Maximilian *(Clinic for Orthopaedics, Trauma and Reconstructive surgery, RWTH Aachen University Hospital)*
Blomeyer, Nadja *(Institute for General Mechanics, RWTH Aachen University)*
Brandl, Christopher *(Institute of Industrial Engineering and Ergonomics, RWTH Aachen University; Department of Product and Process Ergonomics, Fraunhofer Institute for Communication, Information Processing and Ergonomics FKIE)*
Topol, Heiko *(Institute for General Mechanics, RWTH Aachen University)*
Markert, Bernd *(Institute for General Mechanics, RWTH Aachen University)*
Stoffel, Marcus *(Institute for General Mechanics, RWTH Aachen University)*

Acute low back pain (LBP) is thought to have a favorable prognosis; however, when LBP becomes chronic, it contributes to disability and high costs [1]. The intervertebral disc (IVD) is considered to be one of the main etiologies of chronic LBP [2]. Changes in the biomechanical properties of the spine, especially in the intervertebral disc (IVD), are related to multiple factors such as type and duration of loading, recovery periods, osmosis, relaxation, and diffusion processes [3,4]. To quantify spinal burden *in vivo*, various dose models have been developed [5,6].

Both an *in vivo* and *in vitro* study were conducted to investigate the effects of loading and rest periods on the change in mechanical properties of the spine. The *in vivo* study was designed aiming to collect data on physical stress and strain during a lifting scenario. A multi-body simulation (MBS) was used to translate the collected motion data into forces and moments. The Institute of General Mechanics at RWTH Aachen University has developed a test rig for conducting mechanical *in vitro* experiments on spinal cadavers [7,8]. Here, an axial compression force and pure moment loading in flexion/extension, lateral bending, and axial rotation can be applied according to the conditions that have been determined in the MBS. Bovine spine segments are tested in a liquid environment at body temperature with additives as protease inhibitors. According to the sequence of the lifting task, moments are applied in the direction of flexion and extension cyclically on the one hand, and on the other hand, axial compression is exerted in order to represent rest periods. The range of motion of the spinal segments is measured by a magnetic tracking system and the pressure in the *nucleus pulposus* by a fiber-

optic pressure measurement system. Compared to the *in vivo* study, a longer exposure duration is selected in order to investigate its influence on the measured variables. At the end of the experimental period, an endurance test is conducted to provoke damage.

The experimental setup and first results are presented. Findings can be used to optimize ergonomic assessment methods.

References

[1] J.M. Stevans, A. Delitto, S.S. Khoja, C.G. Patterson, C.N. Smith, M.J. Schneider, J.K. Freburger, C.M. Greco, J.A. Freel, G.A. Sowa, A.D. Wasan, G.P. Brennan, S.J. Hunter, K.I. Minick, S.T. Wegener, P.L. Ephraim, M. Friedman, J.M. Beneciuk, S.Z. George, R.B. Saper, JAMA Netw. Open **4**(2), e2037371 (2021).

[2] M.J. DePalma, J.M. Ketchum, T. Saullo, Pain Med. **12**(2), 224-233 (2011).

[3] W. Ehlers, N. Karajan, B. Markert, Biomech. Model. Mechanobiol. **8**(3), 233-251 (2009).

[4] H. Heneweer, F. Staes, G. Aufdemkampe, M. van Rijn, L. Vanhees, Eur. Spine J. **20**(6), 826-845 (2011).

[5] R. Wells, D. van Eerd, G. Hägg, Scand. J. Work Environ. Health **30**(3), 179-190 (2004).

[6] L. Johnen, A. Mertens, V. Nitsch, C. Brandl, Proc. Int. Ergon. Assoc., 93-100 (2021).

[7] K. Brenzel, N. Blomeyer, L. Johnen, M. Praster, M. Rörig, H. Topol, C. Brandl, B. Markert, M. Stoffel, Proc. Appl. Math. Mech. (2023), (Accepted Manuscript).

[8] N. Wilmanns, A. Beckmann, L.F. Nicolini, C. Herren, R. Sobottke, F. Hildebrand, J. Siewe, P. Kobbe, B. Markert, M. Stoffel, J. Biomech. Eng. **144**(7), 71001 (2022).

Gender differences in cycling motions: On objective functions for urban cycling

Schwöbel, Clemens *(3D Cyclelab, Germany)* 10:10
Kelkel, Daniel *(htw saar, Germany)*
Leyendecker, Sigrid *(FAU Erlangen-Nuremberg, Germany)*
Hoffmann, Ramona *(htw saar, Germany)*

Societal challenges such as climate change and the energy crisis are putting bicycles at the center of many people's mobility considerations - but not all. In addition to infrastructure in need of improvement, the stability and comfort while cycling also play a major role. Simulations make it possible to investigate the influence of biometric differences on comfort and stability more cost-effectively than the measurement methods currently used for bike fitting. Bicycle dynamics and multibody simulation of cycling motions have been the subject of research for a long time. Often data-driven models are used that follow pre-established measurement data. Moreover, also optimal control simulations for competitive sports are available, where e.g. the travel distance during a given time is maximised [1]. However, such models are usually based on the biometric data of an average 18-25 year old male, while the influence of gender differences on cycling motions are rarely explored. Yielding towards closing this gender data gap, we use a discrete mechanics and optimal control framework (DMOCC [2]), which benefits from its structure-preserving formulation and has been successfully used for biomechanical applications [3]. The implemented multi-body model of a leg performing a cycling motion can be adapted to individual 3D scans via the geometry parameters and the limits of joint angles and torques, which offers the possibility to investigate the

influence of biometric differences on the resulting motions. In this first approach, we discuss several possibilities to formulate appropriate objective functions for cycling. The final aim of this study is to supplement a given bike frame by software chosen adaptations so that it optimally fits to individual biometric conditions, thus increasing comfort, the sense of safety and performance, which ultimately enables greater participation in the mobility transition for women, children and seniors.

References:

[1] C. Jansen and J. McPhee. Predictive dynamic simulation of Olympic track cycling standing start using direct collocation optimal control. Multibody Syst Dyn, Vol. 49, pp. 53-70, 2020.
[2] S. Leyendecker, S. Ober-Blöbaum, J. Marsden, and M. Ortiz. Discrete mechanics and optimal control for constrained systems. Opt Contr Appl Met, Vol. 31, pp. 505-528, 2010.
[3] R. Hoffmann, B. Taetz, M. Miezal, G. Bleser and S. Leyendecker. On optical data-guided optimal control simulations of human motion. Multibody Syst Dyn, pp. 1-22, 2019.

S02-05: Biomechanics

Date: June 2, 2023 11:00-13:00
Room: POT/351

Chemo-electro-mechanical modelling of the stress corrosion cracking in biodegradable magnesium-rare earth alloys

Zhang, Dawei *(RWTH Aachen University, Germany)* 11:00
Ma, Songyun *(RWTH Aachen University, Germany)*
Markert, Bernd *(RWTH Aachen University, Germany)*

Biodegradable magnesium alloys have emerged as a next-generation material in biomedical applications due to their excellent mechanical properties, biocompatibility, and biodegradability. Their similar mechanical properties to human bone tissues help to avoid stress shielding during the bone healing process. More attractively, the biodegradability of magnesium alloys in human body eliminates the need for a second surgery and thus reduces the pain of patients and the burden on social healthcare system. However, high corrosion rates of magnesium implants in physiological environments and fast mechanical degradation are still critical issues to be addressed. The addition of rare earth (RE) elements increases the migration resistance of the Mg^{2+} cation and retards its hydration process, leading to a remarkable enhancement of the corrosion resistance of magnesium alloys. In this context, multiphysics modelling and simulation of the effect of Mg-RE phases on the degradation behaviour will facilitate the design of the magnesium-rare earth alloy system. In this study, we develop a phase-field method for modelling stress corrosion cracking in magnesium alloys, considering the chemo-electro-mechanical coupling effect. Quantitative computational analysis is performed to study the influence of grain size and distribution of Mg-RE phases on the local galvanic corrosion and crack propagation. The evolution of corrosion interface morphologies and electric fields will be discussed in detail.

Computational modeling of a coated piezoelectric scaffold

Badali, Vahid *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany; Julius Wolff Institute, Berlin Institute of Health, Charite – Universitaetsmedizin Berlin, Germany)* 11:20
Checa, Sara *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany; Julius Wolff Institute, Berlin Institute of Health, Charite – Universitaetsmedizin Berlin, Germany)*
Zehn, Manfred *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany)*
Marinkovic, Dragan *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany)*
Mohammadkhah, Melika *(Department of Structural Mechanics and Analysis, Institute of Mechanics, Technische Universität Berlin, Germany)*

Over the recent decades, piezoelectric scaffolds have been investigated for their potential to improve bone regeneration. It has been shown that electrical signals generated as a result of the deformation of the scaffold within the body during locomotion are able to stimulate

cells to form bone tissue. However, the design of these scaffolds is not trivial, and experimental trial and error approaches to evaluate the efficacy of piezoelectric scaffolds to support bone regeneration are expensive, time-consuming and ethically questionable. Therefore, our aim is to computationally model piezoelectric scaffolds to investigate the potential of electrical stimulation on bone regeneration. Previously, we have shown that placing piezoelectric patches on the struts of a cylindrical porous scaffold can produce voltages in the range of 10 mV - 30 V, which has been reported to be favourable for bone regeneration. In the present work, a piezoelectric honeycomb like structured scaffold used for the treatment of a 3 cm sheep femoral defect was modelled using finite element techniques. This scaffold has been experimentally shown to enhance bone regeneration [1]. The scaffold is made of electrically inactive Ti alloy, coated with a piezoelectric layer of 0.2 micrometer $BaTiO_3$. The finite element model included the coated scaffold fitted into the bone defect area and a plate and screws to fix the intact bone segments and the scaffold. Piezoelectric properties were assigned to the coating layer of the scaffold and physiological loadings were applied to the bone.

We showed that modeling of an extremely thin layer of coating over the scaffold struts can be achieved using 3D piezoelectric solid elements, however it requires very high computational costs. The generated electric voltage and electric field were computed and compared with the literature in terms of their influence on the bone regeneration process. Novel strategies based on submodeling approaches are required to determine the effect of electrical signals within the scaffold pores (where the cells reside). In the next steps, the effect of electrical stimulation obtained from this scaffold is incorporated into the currently available agent-based bone healing model [2] where migration, proliferation, differentiation and apoptosis as the main cellular activities are defined.

[1] Liu, W., Yang, D., Wei, X., Guo, S., Wang, N., Tang, Z., Lu, Y., Shen, S., Shi, L., Li, X. and Guo, Z., (2020). Fabrication of piezoelectric porous $BaTiO_3$ scaffold to repair large segmental bone defect in sheep. Journal of biomaterials applications, 35(4-5), pp.544-552.

[2] Checa, S., Prendergast, P. J., and Duda, G. N. (2011). Inter-species investigation of the mechano regulation of bone healing: comparison of secondary bone healing in sheep and rat. Journal of Biomechanics. 44, 1237-1245.

Flexoelectric and piezoelectric effects in cortical bone remodelling processes

Witt, Carina *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Leonhard-Euler-Str. 5, D-44227 Dortmund, Germany)* 11:40
Kaiser, Tobias *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Leonhard-Euler-Str. 5, D-44227 Dortmund, Germany)*
Menzel, Andreas *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Leonhard-Euler-Str. 5, D-44227 Dortmund, Germany; Division of Solid Mechanics, Lund University, P.O. Box 118, SE-221 00 Lund, Sweden)*

Under daily activity, human bones frequently undergo micro cracking which causes bone remodelling to take place at a cellular level. These targeted remodelling processes are closely related to (chemo-)electro-mechanical coupling phenomena. To be precise, piezoelectricity as well as flexoelectricity play a role in the initiation of bone remodelling. While the piezoelectric coupling in bone material has already been investigated quite thoroughly, the flexoelectric property of bones has been found more recently [1] and has not been studied as intensively

yet. However, its influence is expected to be significant on small scales since the effect is size-dependent, and large strain gradients are present in the region of micro cracks, and especially at the crack tip.

The impact of both, flexoelectricity and piezoelectricity, on remodelling processes in cortical bone as well as the interplay between these electro-mechanical effects is in the focus of the present contribution. For this purpose, a small bone sample with a narrow micro crack is investigated and size effects stemming from the higher-order characteristic of flexoelectricity are studied. Overall, it is shown how both phenomena can trigger bone remodelling processes by inducing an electric field in response to mechanical stimuli. In the vicinity of the crack tip, where the electric field takes maximum values, this causes mature bone cells (osteocytes) to undergo apoptosis and thereby send out signals to attract the bone cells responsible for remodelling (osteoclasts and osteoblasts).

The entire process including mechanical stimulation, electric field generation, biochemical signalling and, finally, the subsequent bone cell diffusion, is studied in an Isogeometric Analysis framework [2]. Thereby, global C^1-continuity is provided in order to deal with the resulting PDEs up to 4th order. The involved bone cells, i.e. osteocytes, osteoclasts and osteoblasts as well as messenger substances are accounted for by the introduction of additional field variables. Directionally dependent diffusion tensors are used to model the targeted migration of osteoclasts and osteoblasts to the remodelling site. Selected numerical results are presented for each of these simulation steps.

[1] Núñez-Toldrà, R., Vasquez-Sancho, F., Barroca, N., Catalan, G., Investigation of the cellular response to bone fractures: Evidence for flexoelectricity. Sci. Rep. 10, 254, 2020.

[2] Witt, C., Kaiser, T., Menzel, A., Modelling and numerical simulation of remodelling processes in cortical bone: An IGA approach to flexoelectricity-induced osteocyte apoptosis and subsequent bone cell diffusion. J. Mech. Phys. Solids, 173, 105194, 2023.

Modeling of Mechanosensitive Remodeling Processes in Collagen Fibers

Topol, Heiko *(Institute of General Mechanics, RWTH Aachen University, Germany)* 12:00
Stoffel, Marcus *(Institute of General Mechanics, RWTH Aachen University, Germany)*
Markert, Bernd *(Institute of General Mechanics, RWTH Aachen University, Germany)*
Pence, Thomas J. *(Department of Mechanical Engineering, Michigan State University, USA)*

Biological soft tissue is composed of cellular and noncellular components. Living soft tissue undergoes continuous processes of morphological change, for example, in the form of degradation, growth, and remodeling of their constituents. The extracellular matrix (ECM) provides physical and biochemical support in these developments (Topol et al., 2021a). These processes are often initiated or mediated by physical stimuli in static or dynamic form (Stoffel et al., 2017).

Collagen fibers are a main constituent of the ECM in various types of soft tissues. These fibers may undergo breakdown and renewal processes as a part of a collagen remodeling process. Experiments have shown that enzymatic collagen degradation can be slowed down when the fibers are moderately stretched (Flynn et al. 2013; Nabeshima et al. 1996). Mechanical modeling works have taken this effect into account (Jia & Nguyen 2019; Tonge et al. 2015).

The framework by Topol et al. (2021b) accounts for strain-stabilization of collagenous fibers to enzymatic degradation.

If the fiber stretch becomes relatively large by exceeding a certain threshold, then the collagen degradation process is reported to increase again (Ghazanfari et al. 2016; Yi et al. 2016). In our work, we account for this mechanosensitive collagen degradation behavior by proposing a strain energy density function for the fiber in terms of a subassembly of constituents in the fiber cohort. The individual lifespans are governed by a survival kernel that emulates a constant fiber creation rate and a fiber-stretch dependent dissolution rate. The stress-free fiber configuration may differ from that of the fiber-embedding material.

References

B. P. Flynn et al.: Highly Sensitive Single-Fibril Erosion Assay Demonstrates Mechanochemical Switch in Native Collagen Fibrils. Biomech. Model. Mechanobiol., 12: 291-300, 2013

S. Ghazanfari et al.: Modulation of Collagen Fiber Orientation by Strain-Controlled Enzymatic Degradation. Acta Biomater. 35: 118-126, 2016

Z. Jia & T. D. Nguyen: A Micromechanical Model for the Growth of Collagenous Tissues Under Mechanics-Mediated Collagen Deposition and Degradation. J. Mech. Behav. Biomed. Mater. 98: 96-107, 2019

Y. Nabeshima, et al.: Uniaxial Tension Inhibits Tendon Collagen Degradation by Collagenase In Vitro. J. Orthop. Res., 14: 123-130, 1996

M. Stoffel et al.: Towards bioreactor development with physiological motion control and its applications. Med. Eng. Phys., 39:106-112, 2017

T. K. Tonge et al.: Micromechanical Modeling Study of Mechanical Inhibition of Enzymatic Degradation of Collagen Tissues. J. Orthop. Res., 14: 123-130, 2015

H. Topol et al.: On Collagen Fiber Morphoelasticity and Homeostatic Remodeling Tone. J. Mech. Behav. Biomed. Mater. 113: 104154, 2021a

H. Topol, et al.: Fibrillar Collagen: A Review of the Mechanical Modeling of Strain-Mediated Enzymatic Turnover. Appl. Mech. Rev. 73: 050802, 2021b

E. Yi et al.: Mechanical Forces Accelerate Collagen Digestion by Bacterial Collagenase in Lung Tissue Strips. Front. Physiol., 7: 287, 2016.

The numerical treatment of a cell-based mathematical model of tissue regeneration

Grosjean, Elise *(Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany)* 12:20

Simeon, Bernd *(Rheinland-Pfälzische Technische Universität Kaiserslautern-Landau, Germany)*

We are working on the simulations of a PDE-ODE system modeling the dynamics of two cell populations (adipose derived stem cells and chondrocytes) involved in the production of cartilage tissue. They are supposed to migrate, proliferate, and differentiate within an artificial scaffold impregnated with a chemoattractant and contained in a perfusion chamber. Our aim is to identify the parameters of interest. In this context, several methods exist. When dealing with discretized solutions of parameter-dependent PDEs, the sensitivities with respect to

certain parameters of interest may be directly computed from the original problem but it requires solving a new system for each parameter of interest. Thus, when dealing with a large number of parameters, the adjoint method may be a good alternative [1]. We will present an efficient way of combining reduced basis techniques [2] and the computation of the sensitivities with these methods in order to further reduce the computational time. This adaptation will be numerically illustrated with several results on our model problem with finite elements.

[1] JF. Sykes and JL. Wilson, Adjoint sensitivity theory for the finite element method, Finite Elements in Water Resources, Springer, p3-12, 1984.
[2] E. Grosjean and B. Simeon, The non-intrusive reduced basis two-grid method applied to sensitivity analysis, arXiv preprint `https://arxiv.org/abs/2301.00761`, 2023.

S03: Damage and fracture mechanics

Organizer(s): **de Lorenzis, Laura** *(ETH Zürich)*
Steinmann, Paul *(FAU Erlangen-Nürnberg)*

S03-01: Damage and fracture mechanics

Date: May 30, 2023 13:30-16:10
Room: HSZ/H04

An enhanced phase field framework for cohesive fracture

Lammen, Henning *(TU Dortmund, Germany, Institute of Mechanics)* 13:30
Mosler, Jörn *(TU Dortmund, Germany, Institute of Mechanics)*

Cohesive zone models are very promising for dealing with non-linear fracture mechanics. In contrast to brittle fracture, the Helmholtz energy of cohesive zone models depend on the crack opening. This leads to tractions across the crack, i.e., traction-separation-laws. The two probably important characteristics of a cohesive fracture model are the material's strength and the fracture energy.

With regard to the finite element implementation of cohesive zone models, at least two classes of methods have been established. On the one hand, discrete interfaces can be introduced either as interface elements between the bulk elements or directly within bulk elements (XFEM). On the other hand, cracks can also be approximated as diffuse interfaces with finite thickness. The phase-field method falls into the latter class.

A phase-field approach for cohesive fracture was recently presented by Conti et al. [1] and numerically investigated by Freddi and Iurlano [2]. In contrast to other phase field approaches for cohesive fracture, Gamma-convergence of this models was proven.. Within this talk, the phase field model by Conti et al. [1] will be extended. In particular, the following generalizations are discussed:

- a geometrically exact setting,
- arbitrary hyperelastic material models,
- independent material parameters for the bulk material and the interface (including the material's strength and the fracture energy of the interfaces)
- the introduction of the Microcrack-Closure-Reopening (MCR) effect (cracks only evolve under tensile stresses)

[1] S. Conti and M. Focardi and F. Iurlano, Phase field approximation of cohesive fracture models, Annales de l'Institut Henri Poincaré C, Analyse non linéaire 33 (2016) 1033-1067.
[2] F. Freddi and F. Iurlano, Numerical insight of a variational smeared approach to cohesive fracture, Journal of the Mechanics and Physics of Solids 98 (2017) 156-171.

Numerical 3D-bifurcation analysis of star-shaped crack patterns using the energy method

Jesch-Weigel, Nico *(Technische Universität Dresden, Germany)*
Hofmann, Martin *(Technische Universität Dresden, Germany)*
Wallmersperger, Thomas *(Technische Universität Dresden, Germany)*

13:50

During the drying of ceramic precursors or colloidal gels in glass tubes, star-shaped crack patterns form [1, 2, 3]. As the inhomogeneous drying field advances, the cracks grow stationary. Cracks are left behind as the drying field penetrates further. Starting from four cracks, one or two cracks may then stop. The parameters at which the cracks stop can be found by an equilibrium analysis based on the global mechanical potential. For this, it is necessary to combine the fracture mechanics with a stability analysis (bifurcation analysis) [4]. The number of first and second derivatives of the mechanical potential is minimized by describing the crack front with a Fourier series [5]. The Fourier coefficients are determined under the condition of steady-state crack growth using a gradient method. Eigenvalue analysis is then used to find the parameter set at which the equilibrium position branches (bifurcation point). In addition, the bifurcation contour is used to determine which cracks remain. The derivatives are determined using the Finite Difference method. The mechanical potential is calculated by a linear elastic three-dimensional Finite Element simulation. By exploiting symmetries, the size of the FE model is reduced.

References:

[1] Gauthier, G.; Lazarus, V.; Pauchard, L., Alternating crack propagation during directional drying, Langmuir, 23, 4715-4718 (2007)
[2] Gauthier, G.; Lazarus, V.; Pauchard, L., Shrinkage star-shaped cracks: Explaining the transition from 90 degrees to 120 degrees, Europhys. Lett., 89, 26002 (2010)
[3] Maurini, C.; Bourdin, B.; Gauthier, G.; Lazarus, V., Crack patterns obtained by unidirectional drying of a colloidal suspension in a capillary tube: experiments and numerical simulations using a two-dimensional variational approach, Int. J. Fract., 184, 75-91 (2013)
[4] Jesch-Weigel, N.; Zielke, R.; Hofmann, M.; Wallmersperger, T., Analysis of 3D crack patterns in a free plate caused by thermal shock using FEM-bifurcation, Int. J. Fract. (2023)
[5] Anderssohn, R.; Hofmann, M.; Bahr, H.-A., FEM-bifurcation analysis for 3D crack patterns, Eng. Fract. Mech., 202, 363-374 (2018)

An adaptive time-discretization method for phase-field damage models with discontinuous crack evolution

Rörentrop, Felix *(TU Dortmund University, Germany)*
Mosler, Jörn *(TU Dortmund University, Germany)*

14:10

The modelling of damage behaviour has been an intensively researched topic for decades - both from the mechanical as well as from the mathematics point of view. Since the modelling of sharp cracks/interfaces and the resulting free boundary problem has been shown to be numerically very challenging, phase-field theories have become very popular, cf. [1]. Within this talk, the focus is on rate-independent damage models and their implementation. In this case, the resulting phase-field approximation is characterized by (incrementally defined) non-convex optimization problems. This non-convexity leads to two problems addressed here: 1.

A discontinuous evolution of the crack in time (so-called brutal crack growth) might occur. Therefore two different internal time-scales have to be considered and modeled. 2. Different mathematical solution concepts are applicable to these kinds of rate-independent systems which are generally not equivalent, for instance the concepts of global energetic solutions and balanced viscosity solutions are here to be named. In combination with a time-discrete numerical approximation it is necessary to prove the convergence to one of the solutions concepts, see [2]. Furthermore these approximations have to be carefully evaluated with respect to the predicted physics. One mathematically sound concept bridging the different, aforementioned time-scales is the time-discrete scheme proposed by Efendiev & Mielke, cf. [3]. Within this talk, the framework [3] is implemented into the Finite-Element-Method and carefully analysed from a physics point of view, see [4]. Particularly, the implementation and effect of the different norms and time-increments in the framework [4] are investigated by the means of numerical experiments.
This is a collaborative work together with S. Boddin and D. Knees from the University of Kassel.

References:
[1] B. Bourdin, G.A. Francfort, J-J. Marigo, Numerical experiments in revisited brittle fracture, Journal of the Mechanics and Physics of Solids, 2000, 48, 797-826.
[2] D. Knees, Convergence analysis of time-discretisation schemes for rate-independent systems, ESAIM: Control, Optimisation and Calculus of Variations 2019, 25.
[3] M. A. Efendiev, A. Mielke, On the Rate-Independent Limit of Systems with Dry Friction and Small Viscosity, Journal of Convex Analysis, 2006, 13, 151-167.
[4] S. Boddin, F. Rörentrop, D. Knees, J. Mosler, Approximation of balanced viscosity solutions of a rate-independent damage model by combining alternate minimization with a local minimization algorithm, arXiv preprint https://arxiv.org/abs/2211.12940 2022

An adaptive acceleration scheme for phase-field modelling of high-cycle fatigue

Heinzmann, Jonas *(Computational Mechanics Group, Institute for Mechanical Systems, ETH Zurich)*
Carrara, Pietro *(Computational Mechanics Group, Institute for Mechanical Systems, ETH Zurich)*
Mirzaei, Amir Mohammad *(Department of Structural, Geotechnical and Building Engineering, Politecnico di Torino)*
De Lorenzis, Laura *(Computational Mechanics Group, Institute for Mechanical Systems, ETH Zurich)*

14:30

Phase-field models for fatigue fracture, e.g. [1,2], represent a versatile approach capable of reproducing the main characteristics of fatigue behavior. However, the associated computational effort makes the cycle-by-cycle analysis of components in the high cycle fatigue (HCF) regime with cycle counts $n > 10^4$ - 10^5 practically unfeasible. To overcome this, a cycle-jump acceleration can be adopted, where the explicit cycle-by-cycle resolution of a certain number of cycles Δn is skipped by instead extrapolating selected state variables based on their evolution during only some explicitly computed cycles in between the cycle jumps. To exploit the full potential of this strategy, an adaptive cycle-jump algorithm is proposed for the model presented in [1] which degrades the fracture toughness of the material as a representative

fatigue history variable accumulates above a certain threshold. In the proposed scheme, the core idea lies in deciding when and how many cycles can be skipped based on the cycle-wise rate of a scalar variable Λ which is representative of the fatigue lifetime advancement. For this, the fatigue life of a component is divided into three stages: (1) an initial stage before fatigue effects are triggered, (2) the crack nucleation stage, and (3) crack propagation (including the Paris regime) ending with failure of the component. The representative variable Λ is suitably defined within each of the stages according to their specific features. The behavior and reliability of the proposed cycle-jump scheme is first demonstrated by comparing cycle-by-cycle with accelerated results. Then, the adaptive cycle-jump scheme is used to analyze the fatigue life of various virtual specimens. Finally, the obtained accuracy and speedup are compared with those from other available cycle-jump approaches.

[1] Carrara, P., Ambati, M., Alessi, R. and de Lorenzis L., A framework to model the fatigue behavior of brittle materials based on a variational phase-field approach Comp. Meth. App. Mech. Eng. 361 (2020).
[2] Alessi, R., Vidoli, S., and de Lorenzis, L., A phenomenological approach to fatigue with a variational phase-field model: The one-dimensional case Eng. Frac. Mech. 190(1) (2018) 53-73.

A Hierarchical Sequence based Rank-One Convexification Algorithm with Linear Complexity for a Special Class of Functions.

Köhler, Maximilian *(Chair of Continuum Mechanics, Ruhr-Universität Bochum)*
Neumeier, Timo *(Institute of Mathematics, University of Augsburg, Germany)*
Peter, Malte A. *(Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg, Germany)*
Peterseim, Daniel *(Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg, Germany)*
Balzani, Daniel *(Chair of Continuum Mechanics, Ruhr-Universität Bochum)*

14:50

Relaxation of variational models by replacing an underlying non-convex generalized energy density by a semiconvex envelope is a promising regularisation technique mainly due to two reasons: first, the relaxation by special semiconvex hulls represents the homogenization of microstructures and second, no additional length scale related parameters need to be introduced. The relaxation by rank-one convex hulls is attractive because alternatives like quasi- or polyconvex hulls are difficult and expensive for general problems. However, all techniques for numerically constructing such a rank-one convex hull have a complexity of at least O(N^(d^2)). Therefore, numerical relaxation is infeasible in three dimensions and only possible in special cases in two dimensions if extended algorithms are considered, cf. [1]. Most rank-one convexification algorithms have relied on the mathematical characterization of iterative lamination, which approaches the rank-one convex hull in the limit. However, an equivalent characterization was introduced by [2,Definition 5.14] in terms of hierarchical sequences (H-sequences). In this talk, we will use the H-sequence characterization to construct binary lamination trees in O(t*N), where t is a small integer chosen by the user. This allows us to relax continuum mechanical examples in two and three dimensions by utilizing their underlying mathematical structure. Furthermore, we discuss how the constraint of GL^+ on the deformation gradient

affects the obtained semiconvex hulls.

[1] Daniel Balzani, Maximilian Köhler, Timo Neumeier, Malte A. Peter, and Daniel Peterseim. Multidimensional rank-one convexification of incremental damage models at finite strains. preprint, https://arxiv.org/abs/2211.14318, 2022.

[2] Bernard Dacorogna. Direct Methods in the Calculus of Variations. Number 78 in Applied Mathematical Sciences. Springer, New York, NY, 2. ed edition, 2008.

Evaluation of effective mechanical properties of particle reinforced composites via numerical simulations of representative volume elements

Zanardi, Heloísa *(University of Sao Paulo, Brazil)* 15:10
Schiavon, Fernando Luis *(Federal Institute of São Paulo, Brazil)*
Zago, Igor Paganotto *(Federal University of São Carlos, Brazil)*
Angélico, Ricardo Afonso *(University of Sao Paulo, Brazil)*

The wide use of composite materials in several fields leads to the need for a solid and complete understanding of their behavior under different loads and conditions. The experimental tests regarding their use in different conditions are time-consuming and costly. In this context, numerical simulations can assist experimental tests in predicting macroscopic mechanical behavior via the analysis of microstructure models. This study develops a model to simulate particle-reinforced composite materials submitted to a temperature variation. The matrix and inclusion materials have different coefficients of thermal expansion, and this mismatch can induce cracks when the composite is submitted to thermal loads. In some cases, the resulting cracks can benefit the material properties, for instance, the damaged material has a lower thermal conductivity, which corroborates with a better performance regarding the thermal insulation applications. However, they also reduce effective mechanical properties, possibly impairing the application of the material. This macroscopic (thermo)mechanical behavior can be evaluated by simulating the composite microstructure and applying a homogenization method. Such simulations are accomplished by the analysis of a representative volume element (RVE) using the finite element method (FEM) and applying periodic boundary conditions (PBC). Herein, the RVEs are periodic and consider a random distribution of composite particles with two volume fractions (15% and 30%). These RVEs were generated employing the Random Sequential Adsorption method. Special attention was given to generating a periodic geometry and a periodic mesh. Two material combinations are investigated, one that leads to radial and another to orthoradial cracks. The type of nucleated cracks depends on the coefficients of thermal expansion mismatch and on the temperature variation. A damage model was implemented using Fortran subroutines to simulate the nonlinear matrix mechanical behavior. Initially, the model without the damage process was validated and showed good agreement with both numerical and experimental results in the literature. For the model considering the damage, the material analyzed was a glass matrix with alumina inclusions, as proposed and experimentally studied by Tessier-Doyen. Numerical simulations were carried out in Abaqus finite element software. The macroscopic elastic properties obtained via numerical simulations agree with experimental results reported in the literature.

A sensitivity analysis was performed to evaluate the influence of damage parameters in the macroscopic material response.

Multiscale modeling of fracture behavior of glassy polymers across molecular and continuum scales

Zhao, Wuyang *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)* 15:30
Pfaller, Sebastian *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*

The fracture of materials is intrinsically a multiscale problem across various spatial and temporal scales. At the crack tip, the behavior at the molecular or atomistic level plays an important role, which cannot be addressed by continuum mechanics. In contrast, the material sample during fracture is subject to macroscopic boundary conditions far away from the crack tip. The mechanisms at the molecular level can be studied by molecular dynamics (MD) simulations. However, due to the limitation of computational cost, it is difficult for MD simulations to capture the fracture behavior of the whole material sample with appropriate boundary conditions. Instead, multiscale modeling of fracture is required that can cover these different scales, where only the crack tip is treated at the atomistic or molecular scale. The Capriccio method is such an approach designed for multiscale simulations of amorphous polymers coupling a continuum and an MD domain in an overlapping region. To facilitate multiscale simulations of glassy polymers at large strains, a viscoelastic-viscoplastic constitutive model that can resemble the mechanical behavior of the material in MD simulations is employed in the continuum domain. With the Capriccio method, we implemented multiscale simulations of the fracture of glassy polymers under various deformation conditions using coarse-grained atactic polystyrene as sample material. Specifically, fracture simulations in mode-I test under plane strain and plane stress conditions as well as three-point bending tests are presented and discussed.

Phase-Field Modeling of Fracture in Polymer Nano-Composites via Graded Interphases

Kumar, Paras *(Instiute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; Competence Unit for Scientific Computing, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)* 15:50
Mergheim, Julia *(Instiute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*

The superior efficacy of nano-particles in enhancing the elastic and fracture behavior of polymers, in comparison to their microsized counterparts, has been demonstrated by numerous experimental observations [1]. A combination of multiple intricate mechanisms, including particle debonding along with branching and merging of several cracks, however, needs to be considered during the numerical modeling of fracture in such unprecedented materials. The phase-field approach to fracture [2], owing to its inherent capability to deal with complex crack topologies in a diffuse manner, has appeared as a viable candidate for modeling crack propagation in heterogeneous materials. Standard phase-field fracture models, however, do not account for interfacial effects which play a crucial role in case of polymer nano-composites. Motivated by experimental observations regarding the existence of an interphase region around the filler particles, we employ the graded-interphase-enhanced phase-field fracture

(PFF-GI) approach proposed in [3]. Herein, a continuous grading of the elastic and fracture properties within a finite thickness interphase region around the inclusions, by means of a physically motivated power-law type interpolation function, is considered. The degree of grading facilitates control over the composite material's fracture behavior and consequently, enables the modeling of a wide spectrum of experimentally observed fracture responses with minimal modification of the standard phase-field fracture approach.

References

[1] M. Quaresimin, M. Salviato and M. Zappalorto, 2015, Toughening mechanisms in nano-particle polymer composites: experimental evidences and modeling Toughening Mechanisms in Composite Materials, Eds. Q. Qin and J. Ye, Woodhead Publishing, 113-133.
[2] B. Bourdin, G. A. Francfort and J.-J. Marigo, 2008, The variational approach to fracture J. Elast. 91(1), 5-148.
[3] P. Kumar, P. Steinmann and J. Mergheim, 2022, A graded interphase enhanced phase-field approach for modeling fracture in polymer composites. Forces Mech., 9, 10013

S03-02: Damage and fracture mechanics

Date: May 31, 2023 08:30-09:30
Room: HSZ/H04

Combining Damage and Fracture Mechanics for the identification of crack propagation parameters

Dray, Samy *(Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS, Gif-sur-Yvette, France; Leibniz University Hanover, Institute of Applied Mathematics, Hanover, Germany)*
Fau, Amélie *(Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS, Gif-sur-Yvette, France)*
Hild, François *(Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS, Gif-sur-Yvette, France)*
Wick, Thomas *(Leibniz University Hanover, Institute of Applied Mathematics, Hanover, Germany; Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS, Gif-sur-Yvette, France)*

08:30

The presentation deals with accurate identification of fracture mechanics parameters inside cracked media using results from damage mechanics simulations. To model damage, a phase-field model was employed based on a variational formulation. This framework allows for parallel computations and mesh refinement with both uniform and locally adapted meshes. The phase-field internal length scale can thus be easily adapted.

A crack opening displacement-controlled virtual test on a beam representative of mortar was studied. The material had a non-negligible fracture process zone size. This means that the crack tip position cannot be precisely determined. In damage mechanics or regularized fracture using phase-field, the crack tip is usually approximated by a smoothed indicator variable. This is a major difference for this type of model compared to fracture mechanics solutions that explicitly deal with (discontinuous) cracks.

The main objective of this study was to combine phase-field with a fracture mechanics model (Williams' series) to extract the crack tip position from the simulations in addition to the fracture energy and the fracture process zone size. In the application, the displacement field resulted from phase-field simulations and was considered to determine the amplitudes of each Williams' field via least squares minimization. The proposed approach accounted for various mesh refinements, as well as the analysis of the numerical and identification residuals.

The results allowed us to conclude about the dependence between the phase-field variable at the crack tip and the internal length at any loading step. This conclusion adds more knowledge and accuracy to usual criteria in damage mechanics that approximate the crack tip position for a fixed damage level.

Employing Miniaturized Test Methods to Determine High-temperature Strength of Carbon-bonded Alumina

Takht Firouzeh, Shahin *(TU Bergakademie Freiberg, Germany)*
Abendroth, Martin *(TU Bergakademie Freiberg, Germany)*
Kiefer, Björn *(TU Bergakademie Freiberg, Germany)*

08:50

Ceramic filters made from carbon-bonded Alumina (Al2O3 − C) are mainly used for the reduction of non-metallic impurities from the metal melt. Considering the extreme applied thermal and mechanical loads, failure behavior analysis of the bulk material at high temperatures is crucial. Ball-on-three-ball test (B3B) is a well-proven test method for this aim, in which a spherical punch loads the disc-shaped specimen until its failure. To employ an alternative test method with higher feasibility, the Brazilian disc test (BDT) was investigated. In this test, the disc-shaped specimen is compressed along its diameter until it splits. To overcome the challenges regarding the application of BDT on fine-grained porous ceramics, a modified version of this test was evolved. With the help of a finite element model, the failure load of Brazilian discs was used to calculate the fracture stress. Obtaining the distribution of stress values at 1200°C and 1500°C, the maximum likelihood method was implemented for the estimation of the Weibull parameters. Apart from observing the high-temperature strength variation of Al2O3 − C, it is aimed to compare the application and results of these two experimental methods. However, due to different specimen geometries, a comparison of the obtained results from B3B and BDT is only possible after the calculation of the volume-related Weibull stress.

Fractures in glaciers – crack tips and their stress fields by observation and modelling

Humbert, Angelika *(Alfred Wegener Institute Helmholtz Centre for Polar and Marine Research, Germany; University of Bremen, Department of Geosciences, Bremen, Germany)*
Gross, Dietmar *(Technical University of Darmstadt, Institute for Mechanics, Division of Continuum Mechanics, Darmstadt, Germany)*
Sondershaus, Rabea *(Technical University of Darmstadt, Institute for Mechanics, Division of Continuum Mechanics, Darmstadt, Germany)*
Müller, Ralf *(Technical University of Darmstadt, Institute for Mechanics, Division of Continuum Mechanics, Darmstadt, Germany)*
Steeb, Holger *(University of Stuttgart, Institute of Applied Mechanics, Stuttgart, Germany)*
Braun, Matthias *(FAU Erlangen-Nürnberg, Institute for Geography, Erlangen, Germany)*
Brauchle, Jörg *(German Aerospace Center, Institute of Optical Sensor Systems, Berlin-Adlershof, Germany)*
Stebner, Karsten *(German Aerospace Center, Institute of Optical Sensor Systems, Berlin-Adlershof, Germany)*
Rückamp, Martin *(Bavarian Academy of Science and Humanities, Section Geodesy and Glaciology, Munich, Germany)*

09:10

Fractures in glaciers are leading to calving of icebergs, to break-up events and disintegration of floating glacier tongues or ice shelves and to drainage of supraglacial lakes. Ice is a brittle material and obeys a viscoelastic rheology of a Maxwell fluid. Areas where elastic strain is large are matching locations where major crevasse fields in outlet glaciers exists. High resolution optical camera systems are opening new opportunities to study fractures in ice. Here we present data obtained from the MACS camera system operated onboard of AWI's polar aircraft in northeast Greenland in 2022. In addition we are using optical and radar satellite imagery. The study area is the 79°N Glacier (Nioghalvfjerdsbræ) is located, that drains more than 6% of the Greenland Ice Sheet. We found that crack tips are exhibiting additional isolated cracks ahead of the main fracture. Subsequent crack propagation is starting from those isolated cracks, leading to an advance of the fracture length, with bridges between crack faces. The bridges provide information of the episodic crack propagation. Fractures have typically a length scale of kilometres and the distance of crack faces is in the order of meters to tenths of meters. Fracture modes will be inferred from stress fields computed by an inverse modelling approach using the Ice-sheet and Sea-level System Model (ISSM). To this end satellite remote sensing derived surface velocity field is used for the optimal control method that constrains model parameters, e.g. basal friction coefficient or rheology. We present a synthesis of imagery of crack tips, the temporal evolution, the stress fields and fracture modes.

S03-03: Damage and fracture mechanics

Date: May 31, 2023 14:00-16:00
Room: HSZ/H04

Ductile damage and failure of thin sheet metals: new biaxial experiments and numerical simulations

Gerke, Steffen *(Universität der Bundeswehr München, Germany)* 14:00
Ramón Valencia, Fabuer *(Universität der Bundeswehr München, Germany)*
Brünig, Michael *(Universität der Bundeswehr München, Germany)*

The presentation deals with the ductile damage and failure behavior of thin sheet metals under proportional biaxial loading paths. Three different newly designed specimens are presented and a experimental series is performed. Corresponding numerical simulations including plastic anisotropy reflect the stress state and enable the interpretation of the different damage mechanisms. Thin sheets with a thickness of 1 mm and less are often characterized by plastic anisotropic behavior which results from their manufacturing process. Consequently, the experimental series has to reflect this aspect, which can be realized, based on the specimen geometry or on the loading conditions. Furthermore, biaxial experiments with suitable specimens can be used to generate wide variety of stress states in a targeted manner and can be applied to investigate the stress-state-dependent damage and failure behavior. Due to fabrication issues the specimen geometry for this class of materials has to get by without notches in thickness direction and in addition stability issues have to be addressed. The new specimens pre-define the localization by a series of holes and a new downholder reduces out-of-plane displacements. The strain fields at the specimen surface are evaluated by digital image correlation at significant points of the loading history. Corresponding numerical simulations considering plastic anisotropic behavior reveal the present stress states and facilitate the analysis of the stress-state-dependent damage and failure behavior. Consequently, the experimental and numerical methods described here provide a possibility for the targeted investigation of the ductile damage behavior of thin sheet metals under proportional loading.

Characterization of ductile damage and fracture behavior under shear reverse loading condition

Wei, Zhichao *(Institut für Mechanik und Statik, Universität der Bundeswehr München, Germany)* 14:20
Gerke, Steffen *(Institut für Mechanik und Statik, Universität der Bundeswehr München, Germany)*
Brünig, Michael *(Institut für Mechanik und Statik, Universität der Bundeswehr München, Germany)*

One-axis-loaded shear monotonic and cyclic tests have shown that the coalescence of the micro-shear-cracks mainly causes ductile damage, and shear reverse loading affects the evolution of damage and fracture behavior compared to the monotonic loading. In the last decades, a limited number of studies have focused on torsion reverse loading under non-

proportional loading condition with cylindrical specimen. In the case of metal sheets, biaxial specimens enable non-proportional loading by changing the tensile preload to shear load during the experiment. In addition, different tensile preloads, without unloading, can generate a variety of stress triaxialities resulting in further damage and fracture under shear reverse loading. To fill this gap, a series of biaxial shear reverse loading with non-proportional loading tests taking into account different tensile preloads is performed for aluminum alloy sheets. In the numerical analysis, an anisotropic cyclic plastic-damage constitutive model is considered to characterize the damage and fracture behavior. Additionally, the change in the hardening rate is observed after shear reverse loading. Thus, a newly modified non-hardening strain region method is introduced to capture the change in the hardening ratio between isotropic and kinematic hardening. Furthermore, the damage surface is assumed to translate in the direction of the damage strain increment. Hence, a softening law based on the damage strain is proposed. The softening material parameters are identified using a unit cell containing a spherical void. The modified constitutive model predicts macroscopic force-displacement and microscopic evolution of plastic and damage behaviors under shear reverse loading with various tensile preloads. Through digital correlation technique and scanning electron microscopy, numerical results can be validated with experimental ones. Furthermore, scanning electron microscopy pictures can also reveal different damage mechanisms on the micro-level.

A non-local damage-plasticity model based on a smooth elastic-plastic transition

Livnoni, Michal *(Technion - Israel of Technology)*
Jabareen, Mahmood *(Technion - Israel of Technology)*
14:40

In the present study, an extension of a smooth inelasticity finite-strain model to include softening and localization based on a strongly over-nonlocal gradient-enhanced formulation is presented. The over-nonlocal formulation includes an intrinsic length parameter, eliminates mesh sensitivity, and allows the model to capture the real mechanical behavior of materials due to localization associated with strain softening. The constitutive equations depend only on quantities that can be measured in the current state of the body, and the transition from elastic to plastic response is smooth. Also, in the present study, a finite element formulation which incorporates three variational fields for the equilibrium equations and an additional field for the Helmholtz type equation for the gradient-enhanced formulation is introduced. The capabilities of the developed finite element to predict occurrence of shear bands and to display mesh-insensitivity are demonstrated by a set of numerical examples.

Gradient-plasticity vs Gradient-damage – What to choose for the Modelling and Calibration of Ductile Damage?

Friedlein, Johannes *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
Mergheim, Julia *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
Steinmann, Paul *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
15:00

Material modelling for metal forming involves large plastic strains and is inherently linked to the evolution of damage. This (plasticity-driven) ductile damage may hide invisibly inside

the material, but can nevertheless affect manufacturing processes and product lifetimes. The modelling and identification of this process-induced damage is conducted by means of a fully coupled plasticity-damage continuum material model at finite strains. We contrast different approaches for gradient-enhancement to regularise the coupled problem. This comprises "plasticity - gradient-damage", where the gradient-enhancement is placed on the damage variable, as well as "gradient-plasticity - damage" with a gradient-enhanced plasticity formulation. Further attention is paid to the numerical implementation and identification of the associated internal length.

Based on the gradient-enhancement of the free energy, multiple types of localisation, such as damage and softening plasticity, can effectively be eliminated by the introduction of additional internal length scales. Different variables are studied to insert strong non-locality for plasticity and damage. This choice does not only affect the scope of the regularisation, but also influences the calibration procedure for the material model. For instance, the gradient-enhancement of the damage variable alters the locally prescribed damage evolution, thus for instance a directly identified failure strain is not accurately reproduced. This can complicate inverse parameter identifications, which are especially tedious when many experiments need to be considered simultaneously, e. g. for coupled stress-state dependent damage models. For damage identification, global force responses together with local deformation measurements are utilised to improve the uniqueness of the optimisation problem.

Experiments and numerical examples demonstrate the regularising capabilities and characteristics of the gradient-plasticity approach and the gradient-damage approach. Moreover, further insights into the regularisation and its requirements are presented, which will become evident in the conducted parameter identification for sheet metal.

Analysis of effects of material anisotropy on ductile damage using microscopic unit cell-model

Koirala, Sanjeev *(Universität der Bundeswehr München, Germany)*
Gerke, Steffen *(Universität der Bundeswehr München, Germany)*
Brünig, Michael *(Universität der Bundeswehr München, Germany)*

15:20

It is experimentally observed that the failure in ductile metals is mainly due to the nucleation, growth and coalescence of micro-voids as well as micro-shear-cracks. Furthermore, plastic anisotropy has significant role in damage and failure behavior of ductile metals. Finite element simulations of unit cell provide a basis to understand different mechanisms on micro-scale for example changes in shape and size of single voids and defects as well as localization of plastic strains. This contribution deals with the numerical analysis of unit cell containing spherical void subjected to symmetrical boundary conditions taking material anisotropy into account. Elastic isotropic behavior is described by Hooke's law while Hoffman yield criterion considering the strength-differential effect is used to model the anisotropic plastic behavior. The anisotropic material parameters are obtained by conducting tensile, compression and shear tests in different directions with respect to the rolling direction. Generalized anisotropic stress invariants, generalized stress triaxiality and generalized Lode parameter are introduced to characterize the stress state in the anisotropic ductile metal. The effect of

plastic anisotropy on the damage behavior of aluminum alloy EN AW-2017A is studied in detail by performing a series of numerical simulations covering a wide range of stress triaxialites and Lode parameter. Stress triaxility and Lode parameter are controlled and kept constant during the entire loading process. The numerical results are then used to discuss general mechanisms of damage and failure process in ductile metals. In addition, damage strains evolution equation is proposed and different stress-state-dependent parameters of damage evolution equation is identified using the results of numerical simulations.

Limitations and possibilities of (an-)isotropic ductile damage models in metal forming

Feike, Klas *(TU Dortmund University, Institute of mechanics, 44227 Dortmund Germany)*
Langenfeld, Kai *(TU Dortmund University, Institute of mechanics, 44227 Dortmund Germany)*
Kurzeja, Patrick *(TU Dortmund University, Institute of mechanics, 44227 Dortmund Germany)*
Mosler, Jörn *(TU Dortmund University, Institute of mechanics, 44227 Dortmund Germany)*

15:40

The prediction of damage and failure is still one of the most fundamental challenges in engineering. It connects to the efficient use of resources as well as to recent developments of simulation frameworks [1,2]. A particular impact, for instance, is on forming technology due to the large plastic deformations and the demanding operational conditions of modern machinery.

Constitutive models are frequently applied in order to predict the onset and the evolution of damage in simulations. As a compromise between accuracy and practicability, many models do not use the entire stress state for damage determination, though. A frequently applied class of such models is based on the triaxiality and the lode parameter of the respective stress state. While such an isotropic approximation indeed leads to a better interpretation and efficiency, damage is usually characterized by an anisotropic degradation of the material. As a consequence, the aforementioned isotropic approximation shows certain limitations, cf. [3].

The present analysis will discuss under what conditions triaxiality and the lode parameter can become insufficient for the characterization of damage evolution. The basis is an anisotropic ductile damage model [4]. Analyses on a material point level reveal loading paths, for instance, that lead to less damage evolution, despite having a higher triaxiality – in contrast to established isotropic models, cf. [5].

[1] Langenfeld, K. and Mosler, J. (2019). A micromorphic approach for gradient-enhanced anisotropic ductile damage. Computer Methods in Applied Mechanics and Engineering 360. 112717.
[2] Clausmeyer, T. et al. (2020). Prediction of Ductile Damage in the Process Chain of Caliber Rolling and Forward Rod Extrusion. Procedia Manufacturing 47. 649-655
[3] Chow, C.L. and Lu, T.J. (1989). On the evolution laws of anisotropic damage, Engineering fracture mechanics 34. 679-701.

[4] Ekh, M. et al. (2003). Anisotropic damage with the MCR effect coupled to plasticity. International Journal of Engineering Science 41. 1535-1551.
[5] Malcher, L. and Andrade Pires, F. (2011). An assessment of isotropic constitutive models for ductile fracture under high and low stress triaxiality. International Journal of Plasticity. 30-31.

S03-04: Damage and fracture mechanics

Date: June 1, 2023 08:30-10:30
Room: HSZ/H04

An anisotropic damage model for finite strains with full and reduced regularization of the damage tensor

van der Velden, Tim *(RWTH Aachen University, Institute of Applied Mechanics, Germany)* 08:30
Holthusen, Hagen *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*
Brepols, Tim *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*
Reese, Stefanie *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*

The modeling of damage as an anisotropic phenomenon enables the consideration of arbitrarily oriented microcracks at the material point level. Yet, the incorporation of material softening into structural simulations still requires a regularization of e.g. the degrading variable. There exist different possibilities for a regularization in case of anisotropic damage with varying numbers of nonlocal degrees of freedom corresponding to e.g. the symmetric integrity tensor [1], the principal traces of the damage tensor [2] or a scalar damage hardening variable [3]. Here, we propose a finite strain formulation with a symmetric second order damage tensor of which all six independent components are regularized with a corresponding nonlocal degree of freedom. Due to the significant increase in computational cost caused by the full regularization of the damage tensor, alternative approaches for a reduced regularization with fewer nonlocal degrees of freedom are presented. Thereafter, the results of the condensed technique are compared to the reference solutions of the model with full regularization.

[1] Langenfeld, K., Mosler, J., 2020. A micromorphic approach for gradient-enhanced anisotropic ductile damage. Comput. Methods Appl. Mech. Eng. 360, 112717.
[2] Holthusen, H., Brepols, T., Reese, S., Simon, J.-W., 2022. A two-surface gradient-extended anisotropic damage model using a second order damage tensor coupled to additive plasticity in the logarithmic strain space. J. Mech. Phys. Solids 163, 104833.
[3] Fassin, M., Eggersmann, R., Wulfinghoff, S., Reese, S., 2019. Gradient-extended anisotropic brittle damage modeling using a second order damage tensor - Theory, implementation and numerical examples. Int. J. Solids Struct. 167, 93 - 126.

On the predictive capabilities of nonlocal models for ductile crack propagation under different levels of stress triaxiality

PHAM, RINH DINH *(TU Bergakademie Freiberg, Germany)* 08:50
El Khatib, Omar *(TU Bergakademie Freiberg, Germany)*
Hütter, Geralf *(TU Bergakademie Freiberg, Germany; Brandenburg University of Technology Cottbus-Senftenberg, Germany)*
Seupel, Andreas *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*

Ductile materials are used in many applications such as hydrogen storage and transport, energy plants and additively manufactured components. High safety standards are vital for

such applications, which underline the necessity of thoroughly investigating ductile failure to ensure safety and increase component efficiency. Ductile failure is mainly prompted by the evolution of so-called ductile damage, characterized by the nucleation, growth and coalescence of microvoids due to plastic deformation. Moreover, the plastic zones formed at the crack tip of ductile materials exhibit high sensitivity to the stress triaxiality level, which in turn distinctly depends on the geometry of the considered component. The quantification of the stress triaxiality at the crack tip is therefore essential to better understand and predict ductile crack propagation and failure. For that reason, a nonlocal ductile damage model is employed in this work to simulate the ductile crack propagation under different stress triaxiality conditions. Different geometries are considered, such as constrained geometries of notched bending specimens and unconstrained geometries of center cracked tension specimens, which characterize the different triaxiality levels. To address the effects of thickness and initial crack length, three dimensional geometries are simulated, which account for the out-of-plane crack-tip constraints. Finally, to evaluate the prediction quality of the simulations, corresponding experiments have been carried out and direct comparisons are conducted, w.r.t the crack length, ductile crack propagation and resistance curves.

Multiphase-field modelling of the interactive pitting corrosion and ductile fracture in biodegradable magnesium alloys

Ma, Songyun *(RWTH Aachen University, Germany)* 09:10
Zhang, Dawei *(RWTH Aachen University, Germany)*
Markert, Bernd *(RWTH Aachen University, Germany)*

Biodegradable magnesium alloys have been developed as promising biomedical materials for temporary implants. Understanding and modelling the corrosion behaviour of magnesium alloys under mixed chemo-mechanical loadings will facilitate the development of implant design. To this end, a number of experimental and computational studies have attempted to assess and understand the complex in vitro corrosion and damage mechanisms of different magnesium alloy systems. In this study, a multiphase-field model is proposed based on the variational principle to capture the interactions between pitting corrosion and ductile fracture in biodegradable magnesium alloys. Multiple order parameters are introduced to track the interfaces associated with crack propagation and magnesium dissolution. The deformation-fracture-corrosion interactions are considered in the energetic variational formulation with physics-based coupling functions. The governing equations are discretised using an incremental variational method and solved by a staggered scheme. Parametric studies on the coupling functions are performed to demonstrate the flexibility of the model with different model parameters. The proposed multiphase-field model is calibrated and validated by in vitro experiments with smooth and notched specimens of WE43 magnesium alloy. The experimental and computational results demonstrate that the proposed model can capture the corrosion, deformation and fracture behaviour in the immersion tests and slow strain rate tensile-corrosion tests.

A gradient-extended two-surface damage-plasticity model for geomaterials

Zhang, Jian *(RWTH Aachen University, Germany)*
Brepols, Tim *(RWTH Aachen University, Germany)*
Reese, Stefanie *(RWTH Aachen University, Germany)*
09:30

A gradient-extended two-surface damage-plasticity model based on the Drucker-Prager yield criterion is proposed in the current work, in which the hydrostatic pressure is considered for the failure behavior of pressure-sensitive materials such as geomaterials and some metals. More precisely, using separate damage and plastic yielding criteria and related loading/unloading conditions, damage and plasticity are considered as distinct but strongly coupled physical mechanisms [1,2]. A return mapping algorithm [3] to the smooth portion and the apex of the yielding cone is adopted to implement the Drucker-Prager yield criterion for both compression and tension loading. Moreover, to overcome the pathological mesh-dependence of the simulation results, the 'micromorphic approach' [1, 4] is used as a suitable damage regularization technique. The letter equips the two-surface damage-plasticity model with a gradient extension. Finally, a numerical example will be provided to show the effectiveness of the present model in damage-plasticity simulations of geological materials.

Modeling fatigue at the microscale by a viscous gradient-enhanced damage model

Kök, Hüray Ilayda *(Leibniz Universität Hannover, Germany)*
Junker, Philipp *(Leibniz Universität Hannover, Germany)*
09:50

An fast and robust technique for simulating fatigue at the microscale is presented through a viscous gradient-enhanced damage model. It begins with the theoretical derivation of the model, which employs an extended Hamilton principle for dissipative systems. The dissipation function is defined as homogenous in first and second order, which yields a differential inequality for the damage function. The damage function is used with the balance of linear momentum and the stress to indicate the beginning of damage once the local Helmholtz free energy exceeds the dissipation parameter. Through this method the nonconvex condensed energy is regularized. Therefore, a well-posed problem is generated, which provides results independent of the mesh. The viscosity can then be modified based on the findings of the experiment rather than being utilized for regularization. The coupled system of equations for the balance of linear momentum (partial differential equation) and the field equation for the evolution of damage (partial differential inequality) can be efficiently solved numerically using the neighbored point approach. By combining finite element and finite difference approaches with operator split techniques, it is possible to perform a fast and accurate assessment of the system of equations (FEM and FDM). Finite element findings, presenting how the new approach works are presented after the model's derivation.

An anisotropic gradient-enhanced damage model for low cycle fatigue and the influence of forming-induced pre-damage

Langenfeld, Kai *(TU Dortmund University, Germany)*
Kurzeja, Patrick *(TU Dortmund University, Germany)*
Mosler, Jörn *(TU Dortmund University, Germany)*

10:10

The prediction of failure due to fatigue is still one of the most fundamental challenges in engineering. Focusing on metals subject to low cycle fatigue, failure usually occurs in two stages: (i) nucleation phase and (ii) coalescence phase. Cyclic plastic strains lead to decohesion and nucleation of cracks at the micro level. Subsequently these micro cracks coalesce into macro cracks, cf. [1]. Nowadays several models are available in the literature in order to predict the onset of damage at the macro level. For instance, critical plane approaches are an efficient tool for predicting the lifetime of components and structures subject to proportional load cases [2]. For non-proportional load cases, however, continuum damage mechanics might be a suitable tool in order to consider the interaction between different strain components more accurately. Within the respective models, the criterion for damage initiation is of utmost importance. Within this talk, the damage initiation criterion in [1] is extended by means of the plastic strain amplitude and the dissipation associated with a suitable ductile damage model. This allows to capture the effect of different load amplitudes at the local level as well as to distinguish between different amplitudes of forming-induced damage, e.g., due to prior cold forming.

[1] J. Lemaitre and R. Desmorat. Engineering Damage Mechanics: Ductile, Creep, Fatigue and Brittle Failures. Springer-Verlag Berlin Heidelberg, 2005.
[2] D. Socie and G.B. Marquis. Multiaxial fatigue. Society of Automotive Engineers Warrendale, PA, 2000.

S03-05: Damage and fracture mechanics

Date: June 1, 2023 16:00-19:00
Room: HSZ/H04

3D Fracture Simulations with an eXtended Phase-Field Method (XPFM)

Klempt, Verena *(Technische Universität Dresden, Germany)* 16:00
Krüger, Christian *(Technische Universität Dresden, Germany)*
Loehnert, Stefan *(Technische Universität Dresden, Germany)*

The newly developed eXtended Phase-Field Method (XPFM) is adapted to an application in 3D. The method combines the advantages of both the Phase-Field Method (PFM) and the eXtended Finite Element Method (XFEM).

The PFM employs a smeared crack approach, which introduces a scalar field, the phase-field, indicating the crack. Due to an energy-based formulation, further criteria regarding crack propagation are obviated. Especially in 3D, where complex crack geometries due to branching and coalescence in multiple directions can occur, this method is very convenient in theory. Practically however, the PFM is seldomly applied for 3D problems since the meshes must be adequately fine to be able to accurately reproduce the high gradients of the phase-field and the displacement field. This leads to a high computational effort, which is even amplified in 3D.

The XFEM on the other hand considers a discrete crack. Here, enrichment functions containing supplementary information about the expected solution, i.e. a jump function across the crack, are added to the standard polynomial ansatz. Since the crack is discretised independently of the mesh, much coarser meshes than within the PFM can be employed. The location of the crack is regarded by level-set functions, denoting the signed distance from each point in the domain to the crack and crack front. However in 3D, the accurate calculation of those level-sets can be very complicated.

The XPFM uses the smeared crack approach of the PFM with a transformed ansatz function. The standard polynomial ansatz is embedded within an exponential function, which is derived from the 1D analytical solution. This allows for much coarser meshes than within the standard PFM. Still, the free development of the crack independently of the mesh is not restricted. The phase-field degrees of freedom themselves attain a level-set like property indicating the position of the crack. They are used directly within a displacement enrichment function allowing for high gradients across the crack even within one element. No additional discrete description of the crack position is necessary.

Since the transformed ansatz and the displacement enrichment are non-polynomial functions and the location of the crack is not known a priori, a standard Gaussian integration approach in areas around the crack is not suitable. This is why an adaptive 3D integration scheme is employed. Several simulations are shown, to demonstrate the effectiveness and efficiency of the application of the XPFM in 3D.

Simulation of Fatigue Fracture Processes using an eXtended Phase-Field Method (XPFM)

Krüger, Christian *(Technische Universität Dresden, Germany)*
Klempt, Verena *(Technische Universität Dresden, Germany)*
Loehnert, Stefan *(Technische Universität Dresden, Germany)*
16:20

Fatigue is a prevalent failure mechanism of engineering structures. To avoid fatigue fractures and to estimate the remaining life span of structural elements, numerical models can be employed. A modern simulation technique for such problems is the phase-field method for fracture coupled with a fatigue model. Besides the approximation of the displacements another state variable, the phase-field, is introduced. It indicates the crack position and is used to reduce the stiffness at the crack and the crack front accordingly. For the consideration of fatigue effects, a strain-history depended variable degrading the fracture toughness of the material is added to the approach. Fatigue characteristics like Wöhler-curves and the Paris-law can be reproduced in this way. Crack phenomena like crack initiation, propagation, branching and merging are implicitly handled by the phase-field method. No explicit criteria or crack geometry tracking methods, like the level-set method in the eXtended Finite Element Method (XFEM) are required. In contrast to the XFEM, using the phase-field method a rather fine mesh is necessary to reproduce the steep gradients of the state variables. Nevertheless, it is not possible to describe the crack path completely independent of the mesh size and the mesh orientation if standard finite element discretisations are used.

Recent developments in combining the phase-field method and the XFEM resulted in the eXtended Phase-Field Method (XPFM). This method combines the benefits of both methods. A transformed exponential phase-field ansatz function (based on the one-dimensional analytical solution of the phase-field problem) and, depending on this transformed ansatz, enrichment functions for the displacement field are defined. Hereby cracks can be represented on much coarser meshes independent of the mesh orientation despite the implicit representation of the cracks. This results in a significant reduction of the number of unknowns in the system of equations to be solved in each iteration step.

In this contribution the XPFM is coupled with a fatigue fracture model for the two-dimensional plane strain case. Due to the non-linear transformation and the enrichment functions a non-standard integration scheme has to be applied. The solution process and a convergence criterion to solve the coupled problem is discussed. Characteristic numerical examples are shown to demonstrate the properties of the new method.

Crack Tip Loading Analysis and Crack Growth Simulation with the Virtual Element Method

Schmitz, Kevin *(University of Kassel, Germany)*
Ricoeur, Andreas *(University of Kassel, Germany)*
16:40

To precisely model crack growth, accurate calculations of crack front loading and crack deflection angles are essential. These calculations require solutions of the underlying boundary value problems (BVPs), which are typically obtained by applying numerical methods, e.g., the finite element method (FEM). However, since accuracy and computational cost of the analyses are in general competing aspects, compromises often must be made to generate satisfactory

results in acceptable times. In contrast, the use of more efficient methods, both for the solution of the BVP as well as for the subsequent crack tip loading analyses, can substantially lower the computational effort while maintaining desired accuracies. The virtual element method (VEM) is a fairly new discretization scheme for the numerical solution of BVPs, and can be interpreted as a generalization of the FEM. Since the VEM can handle arbitrary polygonal and polyhedral meshes in a straightforward manner, it provides a higher degree of flexibility in the discretization process than the FEM, which turns out to be profitable in terms of both computing times and accuracy.

In the context of numerical applications of fracture mechanics, the probably most attractive feature of the VEM results from the possibility to employ elements of complex shapes, which may be convex as well as concave. Consequently, crack growth simulations benefit from the fact that incremental changes in the geometry of a crack do not require any remeshing of the structure, but rather crack paths can run through already existing elements. Although the method has already proved to provide an efficient tool for crack growth simulations in plane problems, there is still further research required regarding the efficient and precise evaluation of crack front loading quantities and the extension towards spatial crack problems.

This work aims to discuss aspects of the virtual element method for crack tip loading analyses and crack growth simulations. Classical concepts of numerical fracture mechanics are adopted and implemented in connection with the VEM, carefully investigating and exploiting the advantages and opportunities the new discretization method offers in this regard. Crack growth simulations based on the VEM are performed and results are compared to reference solutions as well as solutions obtained by the FEM.

A boundary element method with novel special crack-tip elements for dynamic interface crack analysis

Chai, Yuyang *(Department of Civil Engineering, University of Siegen, D-57068 Siegen, Germany)*
Gu, Yan *(School of Mathematics and Statistics, Qingdao University, 266071 Qingdao, PR China)*
Zhang, Chuanzeng *(Department of Civil Engineering, University of Siegen, D-57068 Siegen, Germany)*

17:00

This paper investigates the dynamic interface crack problems in linear elastic composite bi-materials under impact loading by means of the boundary element method (BEM). Considering the local asymptotic behavior of the displacement and stress fields at the tip of an interface crack, novel and more appropriate special crack-tip elements for interface cracks in composite bi-materials are developed and implemented into a multi-domain BEM for the accurate calculation of the complex dynamic stress intensity factors (DSIF). The novel special crack-tip elements can properly describe the local asymptotic oscillatory behaviors of the near-tip displacement and stress fields for cracked composite bi-materials. The validity of the proposed scheme is verified by comparing the numerical results provided by the developed multi-domain BEM with reference results in literature. The present BEM enables a direct evaluation of the complex DSIF from the crack-opening-displacements (CODs) as well as from the crack-tip nodal tractions of the novel special crack-tip elements, without the application of the classical

path-independent contour integral method. Numerical results demonstrate that the present BEM based on the novel special crack-tip elements can significantly improve the computational accuracy of the complex DSIF for cracked composite bi-materials even with a relatively coarse mesh.

On the general 2D case of dynamic brittle fracture in a Lattice Boltzmann method for solids

Müller, Henning *(TU Darmstadt, Germany)*
Faust, Erik *(RPTU Kaiserslautern-Landau, Germany)*
Steinmetz, Felix *(RPTU Kaiserslautern-Landau, Germany)*
Schlüter, Alexander *(RPTU Kaiserslautern-Landau, Germany)*
Müller, Ralf *(TU Darmstadt, Germany)*

17:20

In recent years, the development of Lattice Boltzmann methods (LBMs) for solids has gained traction. We have already presented fracture mechanics as a viable application for these methods with the simulation of dynamic mode III crack propagation. The performance of the LBM itself is promising, while the usage of a regular lattice simplifies the modeling of fractures.

Recent advancements in the quest for LBMs for solids - and especially the description of non-conforming boundary conditions - now make it possible to extend crack propagation to the plane strain case with mode I and II crack opening, including growth with non-uniform speed in arbitrary directions.

As a fracture criterion, the configurational force acting on a crack tip is utilized. The definition of the moments of the LBM, which are based on the balance laws of continuum mechanics, make the evaluation of quantities in the material configuration straightforward.

This presentation restates the LBM for plane strain deformation and discusses the general algorithm for the modeling of growing cracks on a regular lattice, as well as the computation of the configurational force. Numerical examples showcase the performance and the capabilities of this method for the modeling of dynamic fractures.

Numerical investigation of multi-particle interactions using the discrete element method

Rotter, Sonja *(Hamburg Universtity of Technology, Germany)*
Düster, Alexander *(Hamburg Universtity of Technology, Germany)*

17:40

With the growing interest in environmental protection, the collision safety of ships is also increasingly becoming the focus of research. In recent years, various design measures as well as the idea of filling the double hull of a ship with granules [1] have been investigated. All these measures are intended to prevent major damage to the ship and thus also to the crew and the environment in the event of a collision. Due to high experimental costs, there is great interest in the possibility of investigating new ideas numerically. For this purpose, the granular material that can be used as filling for double hulls will be investigated numerically. For this purpose, the open-source discrete element (DEM) solver MUSEN [2] is used, which combines the DEM with a bonded particle method (BPM) that allows the simulation of breaking particles. Particle breakage as well as the interaction of multiple particles are of interest, since

energy dissipation during breakage and the possibility of load transfer through the particles is the main idea of this approach.

In previous work, the numerical investigation of single breaking particles with different BPM models has already been discussed [3]. In the course of this investigation, however, it was found that multi-particle simulations are influenced by different parameters as compared to single-particle simulations. These differences are due to the particle interactions. In order to gain a deeper understanding of these differences, uniaxial multi-particle compression tests are investigated experimentally and numerically. The results of these investigations as well as the main influencing parameters and differences between single and multi-particle simulations are presented in this contribution.

[1] Schöttelndreyer, M. (2015): Füllstoffe in der Konstruktion: Ein Konzept zur Verstärkung von Schiffsseitenhüllen. Dissertation, Institut für Konstruktion und Festigkeit von Schiffen, Technische Universität Hamburg-Harburg.
[2] Dosta, M. and Skorych, V. (2020): MUSEN: An open-source framework for GPU- accelerated DEM simulations. SoftwareX, Volume 12, 100618
[3] Rotter S., Woitzik C., Tasdemir S., Dosta M., Düster A.(2022): Numerical investigation of the breakage and crash absorbing behavior of granular materials in ship collisions. In: Proceedings of International Conference on Processes in Natural and Technical Particle-Fluid Systems 2022 in Hamburg/Germany, Veröffentlichungen des Instituts für Geotechnik und Baubetrieb der Technischen Universität Hamburg, Heft 54, S. 37-51.

Peridynamic simulations of Rock Indentation and excavation

Butt, Sahir *(Ruhr University Bochum, Germany)* 18:00
Meschke, Günther *(Ruhr University Bochum, Germany)*

In this study, we present a peridynamic model for rock fracture and apply it to rock excavation processes. The rock indentation represents the fundamental process for mechanical rock fracturing and is widely encountered in rock excavations. To this end, we simulate indentation tests on sandstone, covering a total of six specimen sizes, using a truncated-tip indenter. The validation for the current model is provided using the experimental data for the indentation tests on Gildehaus Sandstone. A qualitative validation relates to the formation of the crushed zone, from which tensile cracks initiate, while a quantitative validation rests on comparing the force-penetration data obtained from the experiments and the simulations. Finally, we use the model to simulate Linear Cutting Machine (LCM) test, where the rock is excavated using a cutting disc of a Tunnel Boring Machine (TBM), while considering various excavation scenarios.

Why develop twice? Integration of continuum mechanical material models in Peridynamics

Willberg, Christian *(German Aerospace Center, Germany)*
Hesse, Jan-Timo *(German Aerospace Center, Germany)*
Pernatii, Anna *(Otto von Guericke University Magdeburg, Germany)*
Gabbert, Ulrich *(Otto von Guericke University Magdeburg, Germany)*

18:20

To harvest the full potential of the peridynamic approach the state-of-the-art material models should be usable without redeveloping or reimplementing them from classical continuum mechanics theory. User materials (UMAT) in finite element codes allow the researchers or engineers to apply their own material routines. Simple interfaces are specified to allow the utilization of material behaviors in software. In order to use these already existing and often validated models with Peridynamics, a UMAT interface is presented. It allows the simplified use of already existing material routines in the peridynamic framework Peridigm. The interface is based on the finite element (FE) software Abaqus UMAT definition and allows the integration of Fortran routines directly into Peridigm. In addition, the same material model implementations are applicable in finite element applications as well as peridynamic simulations. In the presentation the interface is presented and various material models are utilized and compared between Peridynamics and FE methods. The effect of the horizon and non-local boundaries are analyzed and discussed. To harvest the full potential of the peridynamic approach the state-of-the-art material models should be usable without redeveloping or reimplementing them from classical continuum mechanics theory. User materials (UMAT) in finite element codes allow the researchers or engineers to apply their own material routines. Simple interfaces are specified to allow the utilization of material behaviors in software. In order to use these already existing and often validated models with Peridynamics, a UMAT interface is presented. It allows the simplified use of already existing material routines in the peridynamic framework Peridigm. The interface is based on the finite element (FE) software Abaqus UMAT definition and allows the integration of Fortran routines directly into Peridigm. In addition, the same material model implementations are applicable in finite element applications as well as peridynamic simulations. In the presentation the interface is presented and various material models are utilized and compared between Peridynamics and FE methods. The effect of the horizon and non-local boundaries are analyzed and discussed.

Peridynamic framework to model additive manufacturing processes

Hesse, Jan-Timo *(German Aerospace Center (DLR), Germany)*
Willberg, Christian *(German Aerospace Center (DLR), Germany)*
Hein, Robert *(German Aerospace Center (DLR), Germany)*
Winkelmann, Felix *(German Aerospace Center (DLR), Germany)*

18:40

Additive manufacturing (AM) has emerged as a promising solution for creating complex structures and has the potential to revolutionize the way structures are designed and manufactured. Due to process-related uncertainties, structural properties cannot be determined using classic material testing approaches. In this work, we present the implementation of AM into the peridynamic framework. In order to be able to evaluate future process-related uncertainties, the structure will be virtually manufactured and tested. Peridynamics is a non-

local material model that has gained popularity in recent years for its ability to capture the behavior of materials under various loading conditions.

The main challenge of this integration is to preserve the non-local nature of peridynamics while incorporating the layer-by-layer nature of AM. The proposed approach has been tested on a variety of structures and has shown to be capable of accurately capturing the behavior of AM structures. The implementation of AM into peridynamics provides a unique tool for the simulation and optimization of AM structures, which has important implications for engineering design and manufacturing.

In addition, a novel peridynamic mesh generation algorithm was developed, which ensures that the mesh is suitable for peridynamic simulations. Another algorithm for calculating the outer surface area of each layer has also been introduced, allowing for an accurate representation of the layer-by-layer building process in the simulation. These algorithms provide a more comprehensive and efficient solution for simulating AM structures in the peridynamic framework.

S03-06: Damage and fracture mechanics

Date: June 2, 2023 08:30-10:30
Room: HSZ/H04

A viscoelastic phase field model for the fracture of ice

Sondershaus, Rabea *(Technische Universität Darmstadt, Germany)* 08:30
Humbert, Angelika *(Alfred-Wegener-Institut Helmholtz Zentrum für Polar- und Meeresforschung; Universität Bremen)*
Müller, Ralf *(Technische Universität Darmstadt, Germany)*

The phase field method has become established in fracture mechanics for crack initiation as well as crack propagation. It is a variational approach where the sharp crack interface is regularized and therefore smoothed out over a length scale. The crack is represented by a continuous scalar field which varies between 0 and 1 representing the broken and fully intact material, respectively. We apply the phase field method for fracturing in floating glacier tongues and ice shelves. The detachment of icebergs, known as calving, is defining the lateral extent of ice sheets but is poorly understood. A physical calving law has not yet been found, therefore we investigate the usage of the phase field method for calving. The rheology of ice can be described by a viscoelastic Maxwell fluid consisting of a spring representing the elastic contribution and a dashpot embodying the viscous behavior, connected in series. This results in a short term elastic behavior and a long term viscous behavior. We propose a phase field method for fracture in a viscoelastic fluid. Here we present numerical examples mimicking typical situations found at calving fronts at the margins of the ice sheets in Greenland and Antarctica. We give an analysis of the stress states leading to crack formation and test its sensibility to model parameters such as the energy release rate for ice. As this is still a new field we compare different formulations and assess their appropriateness for our purpose.

Modelling of damage and failure within polymeric adhesives

Lamm, Lukas *(Institute of Applied Mechanics, RWTH Aachen University)* 08:50
Pfeifer, Jan Mirco *(Civil Engineering Mechanics, University of Wuppertal)*
Holthusen, Hagen *(Institute of Applied Mechanics, RWTH Aachen University)*
Brepols, Tim *(Institute of Applied Mechanics, RWTH Aachen University)*
Reese, Stefanie *(Institute of Applied Mechanics, RWTH Aachen University)*

Polymeric adhesives are used in a large variety of different engineering applications. When subjected to finite deformations, such adhesives show a variety of different inelastic phenomena. The combination of incompressible, rate-dependent, temperature dependent, hyperviscoelastic material behaviour with negliable plastic deformations yields a unique material response when it comes to damage and fracture of such materials. In this contribution we show an approach to mathematically describe this particular material response in the context of an isotropic continuum damage framework. This model is based on a finite viscoelastic material formulation combined with a Perzyna-type approach to describe the damage evolution equation. With this formulation we are able to describe both damage due to creep and relaxation of the polymer matrix in both a qualitative and quantitative manner. In order to overcome

pathologic mesh dependencies, we adopt the micromorphic approach as described e.g. in [1]. We furthermore use a special Finite Element formulation with reduced integration and hourglass stabilization (see e.g. [2]) to avoid locking phenomena due to the incompressibility of the material within the elastic loading regime. In addition to the theoretical aspects, we investigate the response of the material model under different loading scenarios and compare the results with experimental data.

[1]: T. Brepols, S. Wulfinghoff, S. Reese; International Journal of Plasticity 129; 102635 (2020)
[2]: O. Barfusz, T. Brepols, T. van der Velden, S. Reese; Computer Methods in Applied Mechanics and Engineering 373; 113440 (2021)

A Generalized Phase-Field Approach for Rate-Dependent Failure of Rubber-Like Materials

Açıkgöz, Kemal *(Middle East Technical University, Mechanical Engineering Department, Turkiye)*
Tanış, Bülent Efe *(Middle East Technical University, Mechanical Engineering Department, Turkiye)*
Dal, Hüsnü *(Middle East Technical University, Mechanical Engineering Department, Turkiye)*

09:10

Rubber-like materials are strongly rate-dependent in both their mechanical responses and fracture properties. In this work, a generalized phase-field approach [1,2] is coupled with a finitely nonlinear viscoelastic theory to investigate the rate-dependent fracture of rubber-like materials. The ground-state hyperelastic response is modeled with a compressible extended eight-chain model [3] which micromechanically motivates a second invariant term. For the viscoelasticity, a multiplicative split of deformation gradient into elastic and viscous contributions is then considered. The generalized Maxwell branches utilize compressible eight-chain models for their elastic response. The kinematics of the rheology of the chains is given for a constitutive creep-rate relation. For the fracture problem, a generalized phase-field approach is formulated, where each term of the extended eight-chain model is associated with a history field that tracks the maximum historical energy related to it and a volumetric-entropic separation. The viscous effects are coupled to the fracture problem through addition of total elastic part free energies of the generalized Maxwell branches to the entropic history field. The viscous contribution can be adjusted with a control parameter. In this work, the viscous volumetric effects are neglected. A set of mechanical characterization experiments (uniaxial tension, equibiaxial tension, and volumetric compression) along with creep and relaxation tests are conducted for unfilled SBR. A series of quasi-static and high strain-rate fracture experiments are performed for a special double edge v-notched specimens (vDENT) obtained using special die-cutters. The baseline quasi-static theory is verified through symmetric and asymmetric vDENT experiments, while the viscous theory is verified over the high strain-rate fracture tests and creep/relaxation experiments.

References

[1] Dal, H. & Açıkgöz, K. (2023). A novel phase-field approach to fracture in rubbery polymers part I: Brittle failure in the quasi-static limit. Manuscript in preparation.
[2] Açıkgöz, K. & Dal, H. (2022). A generalized phase-field approach for the failure of rubberlike materials. In Constitutive Models for Rubber XII (pp. 312-320). CRC Press.

[3] Dal, H., Gültekin, O., & Açıkgöz, K. (2020). An extended eight-chain model for hyperelastic and finite viscoelastic response of rubberlike materials: Theory, experiments and numerical aspects. Journal of the Mechanics and Physics of Solids, 145, 104—159

The rate- and temperature-dependent brittle fracture-to-ductile transition of Toffee: Experimental investigation and phase-field modelling

Dammaß, Franz *(TU Dresden, Institute of Solid Mechanics, Germany)*
Kästner, Markus *(TU Dresden, Institute of Solid Mechanics, Germany)*

09:30

For natural materials such as Toffee-like confections, the mechanical behaviour can drastically depend on rate of deformation as well as on temperature. Besides the rate-dependency of the deformation of the bulk material, it is in particular the characteristics of failure that can essentially change when either the loading rate or the temperature are altered. For instance, at room temperature, Toffee-like sugar-based confections can behave extremely brittle at high strain rates, whereas they may be extensively deformed when the rate of deformation is low. Likewise, the behaviour can significantly change when temperature is altered. This phenomenon is referred to as rate- and temperature-dependent brittle-to-ductile transition.

In this talk, a rigorous experimental investigation of the rate- and temperature-dependent deformation and fracture behaviour of a Toffee-like confection is presented. Furthermore, based upon these experimental data, a phase-field description and model-based analysis is carried out within the framework of the recently developed unified energetic model [1, 2]. In particular, it is demonstrated that the inelastic deformation of the bulk and the fracture resistance do both significantly depend on rate of deformation and temperature.

References

[1] Dammaß, F., Kalina, K., Ambati, M. and Kästner, M., 2022, Phase-field modelling and analysis of rate-dependent fracture phenomena at finite deformation, Preprint, `https://arxiv.org/abs/2206.03460`.
[2] Dammaß, F., Ambati, M. and Kästner, M., 2021, A unified phase-field model of fracture in viscoelastic materials, Continuum Mech. Therm., 33(4), 1907-1929

Investigation on Shear Band Formation at High Strain Rates with a Split Hopkinson Bar Setup

Jentzsch, Stefan *(Bundesanstalt für Materialforschung und -prüfung, Germany)*
Stock, Daniel *(Bundesanstalt für Materialforschung und -prüfung, Germany)*
Häcker, Ralf *(Bundesanstalt für Materialforschung und -prüfung, Germany)*
Kindrachuk, Vitaliy *(Bundesanstalt für Materialforschung und -prüfung, Germany)*
Klingbeil, Dietmar *(Bundesanstalt für Materialforschung und -prüfung, Germany)*

09:50

The essence of dynamic failure is closely linked to the formation of adiabatic shear bands (ASB), which result from the localization of shear strain under high deformation speeds accompanied by a rapid temperature increase. The understanding of this phenomenon is crucial for the modelling of high speed production processes as lathing and forming and in view of safety issues when impacts of fast rotating machine components (e.g. aircraft turbine blades) may occur. Our contribution addresses both the experimental evidence and characterization of ASBs due to impact tests at the Split Hopkinson pressure bar (SHPB) setup and the finite element analysis to determine the parameters of the underlying constitutive

model, which is closely related to Johnson-Cook (JC) material model.
The experimental investigations were performed on notched shear specimens made of the fine grained structural steel S690QL. The geometry of the specimens was designed with the aid of finite element simulations of the whole experimental setup. A series of SHPB tests was carried out where i.e. notch offsets and load pulse shapes were varied. SEM micrographs demonstrated the regions of localized shear. Furthermore, the displacements in the regions affected by shear localization were measured with subset-based local Digital Image Correlation (DIC) where normalized cross correlation (NCC) was applied between correlated frames. Although there were restrictions with the resolutions of the high speed camera at the necessary high frame rates, the available resolutions could be proven as appropriated. Therefore, Principal Component Analysis (PCA) methods, contemplating the correlation between the displacement components, were introduced to examine different measurement grid sizes.

We utilized the Abaqus Explicit package with the viscoplastic JC model including damage evolution to simulate the complete experiment encompassing the shear failure of the specimen due to ductile damage. The displacement fields, obtained in the SHPB tests, were considered as an objective to validate and to identify the constitutive parameters with. In view of high computational costs, the finite element model was reduced to sample discretization, whereas the boundary conditions were derived from SHPB test measurements.
Due to the "viscous effect", the model could reasonably reproduce the displacement distribution without meshdependent issues. The limitations were rather in predicting the evolution rate of the local damage variable. The extension of JC model is therefore introduced.

S03-07: Damage and fracture mechanics

Date: June 2, 2023 16:00-18:00
Room: HSZ/H04

Numerical Optimisation of Damage in Forming Processes

Guhr, Fabian *(TU Dortmund University, Germany)* 16:00
Barthold, Franz-Joseph *(TU Dortmund University, Germany)*

Modern processes of metal forming nowadays face a multitude of challenges. For example, the formed parts are required to endure more difficult loading cases while simultaneously being downsized to lessen production cost and weight. This has an effect on, e.g., the safety margins which are taken into account to prevent possible failure. To ensure the safety of those part, possible reasons for failure have to be better understood. One key aspect which can lead to failure is the induced damage during the metal forming process, and as such, one has to understand and lessen the damage accumulation during forming. This can be achieved by varying the set of process parameters for each given process, e.g., in [1] this is achieved by manually changing these parameter sets for the process of full forward rod extrusion, to better the damage properties of the formed specimen.

Since optimisation of forming processes in a manual fashion is very time consuming and requires a very deep understanding of the underlying processes, additional approaches are of interest. Hence, this talk presents a method of utilising numerical optimisation to computationally enhance certain forming processes. By defining damage depending objective functions and constraints one can generate sets of optimal parameters to form parts with reduced damage behaviour. Due to the necessity of contact formulations within the finite-element (FE) simulations, the commercial FE solver Abaqus is used as the underlying software for said simulations. By utilising Python scripting, a method is presented which allows arbitrary problems to be freely optimised. By altering the design of the forming process within its simulation model database (.cae) as wells as extracting the data from the output database (.odb), one is able to completely automate the optimisation process.

The examples of this talk include the optimisation of full forward extrusion, hollow forward extrusion and stretch forming. The first is used to compare the results of the optimisation with the manual derived results from [1], to validate the presented optimisation framework. The concept is then applied to the more complex process of hollow forward extrusion. Therein, the additional mandrel enters as possible change in design. Additionally, stretch forming is optimised by changing the shape of the drawbead, which in turn alters the material flow and therefore the damage induced within the process.

[1] Hering, O., Tekkaya, A. E., 2020. Damage-induced performance variations of cold forged parts. Journal of Materials Processing Technology 279

Numerical investigation of the process-structure-property relationship of remote laser cut CFRP structures

Schmidt, Benjamin *(Institute of Solid Mechanics, TU Dresden, Dresden, Germany)*
Hollmer, Katharina *(Institute of Materials Science, TU Dresden, Dresden, Germany)*
Zimmermann, Martina *(Institute of Materials Science, TU Dresden, Dresden, Germany)*
Kästner, Markus *(Institute of Solid Mechanics, TU Dresden, Dresden, Germany; Dresden Center for Computational Materials Sciense (DCMS), TU Dresden, Dresden, Germany)*

16:20

The mechanical properties of structures made of carbon fiber-reinforced polymers, which have an immense influence on their usability in many areas, are significantly influenced by process-induced damage and material defects inserted during manufacturing. This is true for all manufacturing processes, even if the type of defects differs greatly. In the field of laser cutting the damaged area is called the heat-affected zone and mainly consists of oxidized fiber ends, matrix evaporation zone, and chemical matrix decomposition below matrix evaporation temperature.

The extent of thermally induced damage depends massively on process parameters such as laser power, pause times, laser focusing, and laser spot speed, and can be influenced purposefully by their choice. Experimentally, the investigation of the entire process parameter space, and especially the destructive investigation of the cut structures is hugely time- and cost-intensive. The existence of different, sometimes competing design goals such as the economical efficiency of the cutting process, surface roughness, and optimal mechanical properties complicate the problem. In this contribution, the numerical analysis of the cutting process is presented. Based on a three-dimensional thermal modeling strategy in the finite element software FEAP, the cutting process is described taking into account phase transformations during the evaporation of matrix and fiber. The moving laser spot is modeled as a heat input on the upper side with a Gaussian distribution. The emerging process gas is assumed to absorb a part of the laser power according to the Lambert-Beer law. The influence of various parameters and their combinations on the design goals of the process are analyzed by evaluating various sensitivity measures. The entire input parameter space is systematically searched using a design of experiment. The cutting geometry is of interest too, so ellipses with varying aspect ratios and thus radii and their influences on the resulting heat-affected zone are analyzed.

A thermo-mechanical phase-field fracture model: application to hot cracking simulations in additive manufacturing

Ruan, Hui *(TU Darmstadt, Germany)*
Rezaei, Shahed *(TU Darmstadt, Germany)*
Xu, Bai-Xiang *(TU Darmstadt, Germany)*

16:40

Thermal fracture is prevalent in many engineering problems and is one of the most devastating defects in additive manufactured metals. Due to the interactive underlying physics involved, the computational simulation to predict and analyze such fracture behavior is important but challenging. In this work [1], we propose a thermo-mechanical phase-field fracture

model, which is based on a thermodynamically consistent derivation. The model is applied to simulate the hot cracking in additive manufacturing. Thereby not only the thermal strain but also the solidification shrinkage is considered. As for the thermal profile, both analytical temperature solution and numerical thermal field around the melting pool are taken into account. Based on the latter approach [2], the influence of different process parameters is further studied. The study reveals that the solidification shrinkage strain takes a dominant role in the formation of the circumferential crack, while the temperature gradient is mostly responsible for the central crack. Process parameter study demonstrates further that a higher laser power and slower scanning speed are favorable for keyhole mode hot cracking while a lower laser power and quicker scanning speed tend to form the conduction mode cracking. The numerical predictions of the hot cracking patterns are in good agreement with similar experimental observations, showing the capability of the model for further studies.

A phase-field model for hydrogen-promoted fracture based on a mixed rate-type variational setting

Diddige, Vikas *(TU Bergakademie Freiberg, Institut für Mechanik und Fluiddynamik, Lampadiusstraße 4, 09599, Freiberg)*
Seupel, Andreas *(TU Bergakademie Freiberg, Institut für Mechanik und Fluiddynamik, Lampadiusstraße 4, 09599, Freiberg)*
Roth, Stephan *(TU Bergakademie Freiberg, Institut für Mechanik und Fluiddynamik, Lampadiusstraße 4, 09599, Freiberg)*
Kiefer, Björn *(TU Bergakademie Freiberg, Institut für Mechanik und Fluiddynamik, Lampadiusstraße 4, 09599, Freiberg)*

17:00

Certain metals experience a substantial deterioration in mechanical properties when exposed to a hydrogen environment, an effect termed hydrogen embrittlement. To understand, predict and counteract this hydrogen-assisted material degradation, sufficiently accurate material models are needed. According to the current hypothesis, hydrogen diffusion is driven by gradients of concentration and hydrostatic stress [1]. To capture this, a phase-field model is formulated as a multi-field problem coupling deformation, crack propagation and diffusion to analyze hydrogen-promoted fracture. Here, the displacements, a fracture-related phase-field, the hydrogen concentration, and the chemical potential are considered as primary field variables. Approaches proposed in the literature often use an extrapolation of the hydrostatic stress gradients calculated at the material point level, which appear in the hydrogen flux relation [1]. In order to circumvent this potentially inaccurate extrapolation, the model is recast into a mixed rate-type variational setting [2], where the chemical potential –whose gradient governs the hydrogen flux– and the hydrogen concentration follow from the numerical solution of a saddle point problem. Staggered and monolithic schemes are investigated in this context. A comparative study is conducted to assess the performance of both formulations qualitatively and quantitatively. Moreover, results for several representative boundary value problems are presented to demonstrate the applicability of the developed numerical framework.

[1] Kristensen, P. K., Niordson, C. F., and Martínez-Pañeda, E. (2020). A phase field model for elastic-gradient-plastic solids undergoing hydrogen embrittlement. Journal of the Mechanics and Physics of Solids, 143:104093.

[2] Miehe, C., Hildebrand, F., and Böger, L. (2014). Mixed variational potentials and inherent symmetries of the Cahn-Hilliard theory of diffusive phase separation. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 470(2164):20130641.

Phase-field cohesive modeling of chemo-mechanical fracture in polycrystalline cathode structures of lithium-ion batteries

Chen, Wanxin *(Technischen Universität Darmstadt, Germany)* 17:20
Rezaei, Shahed *(Technischen Universität Darmstadt, Germany)*
Xu, Bai-Xiang *(Technischen Universität Darmstadt, Germany)*

Cathode particles of lithium-ion batteries (LIBs) present inhomogeneous volume changes due to lithium extraction and insertion during charging and discharging processes, which may lead to crack nucleation, propagation, and even fracture of storage particles, yielding detrimental effects on LIBs' capacities and overall cycle life. In order to model and predict the failure process of cathode particles in LIBs, we proposed a chemo-mechanically coupled cohesive phase-field fracture model based on a thermodynamically consistent framework [1]. In particular, the unique mechanical properties of grain boundaries and the resulting potentially complex fracture patterns, i.e., inter- and intra-granular cracks can be recaptured within the unified mathematical framework, instead of characterizing boundary behaviors in an explicitly cumbersome manner, e.g., interface element [2,3]. The theoretical model has been numerically implemented in the context of the multi-fields finite element (FE) method on open source FE packages MOOSE, with applications to the simulations of damage and fracture processes of NMC cathode particles. Extensive numerical examples demonstrate that the proposed model is able to study arbitrarily complex crack patterns due to evolution of Li-ion concentration, which offers predictive insight into key degradation mechanisms of polycrystalline cathode structures.

[1] Bai-Xiang Xu, Ying Zhao, Peter Stein, 2016, Phase field modeling of electrochemically induced fracture in Li-ion battery with large deformation and phase segregation. GAMM-Mitteilungen, 39, 92-109.
[2] Shahed Rezaei, Armin Asheri, Bai-Xiang Xu, 2021, A consistent framework for chemo-mechanical cohesive fracture and its application in solid-state batteries. Journal of the Mechanics and Physics of Solids, 157, 104612.
[3] Yang Bai, David A. Santos, Shahed Rezaei, Peter Stein, Sarbajit Banerjee, Bai-Xiang Xu 2020, A chemo-mechanical damage model at large deformation: numerical and experimental studies on polycrystalline energy materials. International Journal of Solids and Structures, 228, 111099.

Chemo-mechanical damage modeling of polycrystalline secondary active material for batteries

Asheri, Armin *(Volkswagen AG; Technische Universität Darmstadt)*
Rezaei, Shahed *(Technische Universität Darmstadt)*
Glavas, Vedran *(Volkswagen AG)*
Xu, Bai-Xiang *(Technische Universität Darmstadt)*

17:40

One of the challenges regarding the application of high capacity cathode active materials for lithium-ion batteries such as nickel manganese cobalt oxide with high nickel content is the mechanical degradation during the electrochemical cycling. These layered oxide material show anisotropic material properties such as diffusivity and swelling due to the change in lithium concentration. The anisotropic diffusion induced strain formed in the active material during lithiation/ delithiation causes severe mechanical damage at the grain boundaries of polycrystalline active material particles, which results in degradation and capacity loss. In this work, an anisotropic chemo-mechanically coupled model is implemented to investigate the fracture in secondary cathode active material particles using a cohesive zone model. The diffusion, the chemical strain, and also the stiffness of the active material are treated anisotropic. Moreover the effects of the grain size and the orientation of the grains on the chemo-mechanical behavior and fracture in polycrystalline cathode active material are investigated.

S04: Structural mechanics

Organizer(s): **Elgeti, Stefani** *(TU Wien)*
Österle, Bastian *(TU Hamburg-Harburg)*

S04-01: Structural mechanics

Date: May 30, 2023 13:30-16:10
Room: HSZ/AUDI

A total Lagrangian, objective, and intrinsically locking-free Petrov-Galerkin SE(3) Cosserat rod finite element formulation

Eugster, Simon R. *(University of Stuttgart, Germany)* 13:30
Harsch, Jonas *(University of Stuttgart, Germany)*

In this presentation, we present a novel Petrov-Galerkin SE(3) Cosserat rod finite element formulation, which is total Lagrangian, objective, intrinsically locking-free, and parametrized by a minimal number of six coordinates per node. Specifically, the idea of interpolating the nodal orientations using relative rotation vectors, proposed by Crisfield and Jelenić in 1999, is extended to the interpolation of nodal Euclidean transformation matrices with the aid of relative twists; a strategy that arises from the SE(3)-structure of the Cosserat rod kinematics. The discretized equations are structurally simplified by applying a Petrov-Galerkin projection method where the nodal virtual displacements and rotations, as well as the nodal translational and angular velocities are interpolated instead of using the consistent variations and time-derivatives of the introduced interpolation formula.

Assumed natural strain method for an isogeometric solid beam element

Shafqat, Abdullah *(Mechanics of Functional Materials Division, Institution of Materials Science,TU Darmstadt, Germany)* 14:10
Weeger, Oliver *(Cyber-Physical Simulation Group, Department of Mechanical Engineering,TU Darmstadt, Germany)*
Rezaei, Shahed *(Mechanics of Functional Materials Division, Institution of Materials Science,TU Darmstadt, Germany)*
Xu, Bai-Xiang *(Mechanics of Functional Materials Division, Institution of Materials Science,TU Darmstadt, Germany)*

In this contribution, an isogeometric three-dimensional solid-beam finite element for large deformations and rotations with merely displacement degrees of freedom is developed. The finite strain theory and hyperelastic constitutive models are considered and B-Spline and NURBS are employed for the finite element discretization. As in the Lagrangian formulations, also NURBS-based formulations are affected by the non-physical phenomena of 'locking', which constrains the field variables and negatively impacts the solution. To avoid this problem, the assumed natural strain (ANS) method as proposed for IGA solid-shell elements [1], is applied within the context of the solid-beam formulation. The developed ANS-based IGA solid-beam formulation is implemented in MATLAB using the NLIGA framework [2]. The proposed formulation is tested on several single-patch and multipatch benchmark problems

and results are validated with classical beam finite elements and isoparametric solid-beam (Q1STb) elements [3]. The results show that the proposed formulation can alleviate shear and membrane locking and improve the performance of the isogeometric solid beam element. With the developed element, both efficient and accurate prediction of mechanical properties of lattice-based architected materials [4] can be achieved. It inherits the merits of solid elements like flexible boundary conditions but with much higher computational efficiency. [1] J. F. Caseiro, R. A. F. Valente, A. Reali, J. Kiendl, F. Auricchio, R. J. Alves de Sousa. On the Assumed Natural Strain method to alleviate locking in solid-shell NURBS-based finite elements. *Computational Mechanics,*53:1341-1353, 2014. [2] X. Du, G. Zhao, W. Wang, M. Guo, R. Zhang, and J. Yang. NLIGA: A MATLAB framework for nonlinear isogeometric analysis. *Computer Aided Geometric Design,* 80: 101869, 2020. [3] J. Frischkorn, S. Reese. A solid-beam finite element and non-linear constitutive modelling. *Computer Methods in Applied Mechanics and Engineering*, 265:195-212, 2013. [4] O. Weeger. Isogeometric sizing and shape optimization of 3D beams and lattice structures at large deformations. *Structural and Multidisciplinary Optimization*, 65, 2022.

An efficient exact geometrically defined Reissner-Mindlin shell element for analysis of shell structures

Azizi, Nima *(Brandenburg University of Technology Cottbus-Senftenberg, Germany)*
Dornisch, Wolfgang *(Brandenburg University of Technology Cottbus-Senftenberg, Germany)*
14:30

A curved non-isoparametric Reissner-Mindlin shell element is developed for analyzing shell structures. The standard kinematic description of the element requires the calculation of the director vector. To address this demand accurately, similar to isogeometric analysis (IGA), the geometry is defined by utilization of the non-uniform rational B-splines (NURBS) imported directly from CAD files. Then, shape functions of the Legendre spectral element method (SEM) are used to interpolate the displacements. Consequently, the shell director vector and Jacobian of the transformation are calculated properly according to the presented formulation. On the other hand, in Legendre SEM combined with Gauss-Lobatto-Legendre quadrature, the integration points and the element nodes coincide. Thus, the calculation of interpolated director vector at integration points is not necessary. This is the source of either complexity or error in the calculation of proper local nodal systems in IGA shells [1]. Given the condition number of the stiffness matrix in the developed method, super high-order elements can also be used. The validity and convergence rate of the method are investigated and verified through various cases of h- and p-refinement in challenging obstacle course problems

On the use of dual basis functions in explicit dynamics within isogeometric analysis

Held, Susanne *(BTU Cottbus-Senftenberg, Germany)*
Dornisch, Wolfgang *(BTU Cottbus-Senftenberg, Germany)*
14:50

Isogeometric analysis (IGA) is based on higher order polynomials as shape functions. In contrast to standard Finite Element Method (FEM), where also Lagrange basis functions of higher order can be considered, in IGA the shape functions are directly taken from the CAD model.

Usually they are Non-Uniform Rational B-Splines (NURBS), but in addition there is a variety of other splines. The usage of spline based FEM allows efficient computations with a comparatively low number of elements, as increasing the order of NURBS basis functions also improves the convergence rate.

In the field of IGA, high polynomial orders lead to highly accurate computations for structures subjected to static and dynamic loads. The received mass matrices are highly accurate as well, as the basis functions of high order distribute the mass precisely and therefore causing large bandwidths. Thus, for dynamic analysis with huge numbers of time steps IGA routines strongly increase the computational effort in comparison to low order FEM. Taking care of computational efficiency, in explicit dynamics these problems are commonly faced with mass lumping techniques to achieve diagonal mass matrices. The required inversion of the mass matrix is cut down to trivially taking the reciprocal of each entry. Within explicit dynamic calculations the ensuing steps just include matrix vector multiplications, which are clearly less costly and do not require further improvements. A variety of mass lumping schemes have been developed in the constant progression of FEM. Efficient and simple ones as the row-sum technique are commonly applied. Unfortunately, these well-known and established algorithms deteriorate the nicely convergence rates of IGA, when making use of high polynomial orders. Thus, a lumping scheme for dynamic computations relying on higher order basis functions has to be applied to IGA formulations.

The basic concept of this study is to introduce dual basis functions as test functions to IGA element formulations with NURBS shape functions. Implementing dual test functions transfers the initial Bubnov-Galerkin to a Petrov-Galerkin formulation. Hence, non-symmetric stiffness matrices and as effect of the duality, consistent diagonal mass matrices are received. This enforcement on the element level can be easily applied as transformation of global matrices gained from common IGA formulations as the chosen types of dual basis functions are constructed by a combination of the NURBS shape functions. Thus, the implementation to existing codes can be easily done. Numerical examples show the efficiency of the dual approach in comparison to existing techniques.

Simulation of Linear Elastic Structural Elements Using the Petrov-Galerkin Finite Element Method

Zähringer, Felix *(Karlsruhe Institute of Technology, Germany)* 15:10
Betsch, Peter *(Karlsruhe Institute of Technology, Germany)*

The results of Finite Element (FE) simulations performed with structural elements, such as plates, depend strongly on the selected mesh. Especially in the case of highly distorted meshes, large discrepancies between the numerical and the analytical solution can be observed. In the present contribution, it is investigated for the linear elastic case to what extent the Petrov-Galerkin FE method provides a remedy for this mesh sensitivity.
In contrast to the Bubnov-Galerkin method, which is used for most FE formulations, the Petrov-Galerkin method employs different ansatz spaces for the test and trial functions. More precisely, so-called metric shape functions, which are constructed in the physical space, are used as an ansatz for the trial functions, while the approximation of the test functions is still based on the isoparametric concept. It is worth noting that this procedure generally leads to an asymmetric stiffness matrix.

In several works (cf. [1], [2], [3]), Petrov-Galerkin FE formulations have been proposed for the simulation of linear elastic 2D or 3D continua. Numerical investigations show that the developed elements have advantageous properties when simulations are performed with distorted meshes. To what extent the proposed concepts can be transferred to structural elements, such as plates, is analyzed in the present contribution and illustrated by numerical examples.

References

[1] Rajendran S, Liew KM. A novel unsymmetric 8-node plane element immune to mesh distortion under a quadratic displacement field, *Int J Numer Methods Eng*. 2003; 58:1713-1748. https://doi.org/10.1002/nme.836

[2] Xie Q, Sze KY, Zhou YX. Modified and Trefftz unsymmetric finite element models, *Int J Mech Mater Des*. 2016; 12:53-70. https://doi.org/10.1007/s10999-014-9289-3

[3] Pfefferkorn R, Betsch P. Mesh distortion insensitive and locking-free Petrov-Galerkin low-order EAS elements for linear elasticity, *Int J Numer Methods Eng*. 2021; 122(23):6924-6954. https://doi.org/10.1002/nme.6817

S04-02: Structural mechanics

Date: May 31, 2023 08:30-09:30
Room: HSZ/AUDI

Remeshing and data transfer in the finite cell method for problems with large deformations

Sartorti, Roman *(Hamburg University of Technology, Germany)* 08:30
Düster, Alexander *(Hamburg University of Technology, Germany)*

The simulation of complex structures using standard finite element discretization techniques can be challenging since the creation of the boundary conforming meshes for such structures can be time consuming. Therefore, fictitious domain methods are attractive alternatives because the underlying mesh does not have to conform to the boundary. One fictitious domain method is the finite cell method (FCM) [1] where a structured non-geometry conforming Cartesian grid is created and the geometry is then described by a simple indicator function.

When solving nonlinear problems, for example if large deformation shall be considered, broken cells are typically heavily distorted and may lead to failure of the overall solution procedure. To tackle this issue remeshing is applied to proceed with the simulation. In previous publications radial basis functions (RBF) were applied to map the deformation gradient between the different meshes [2]. However, it is not clear whether this is the best way to transfer data during the remeshing procedure. Therefore, we investigate whether there are alternative quantities that can be used instead. This is then compared to the RBF interpolation and applied to different numerical examples with hyperelastic material model under large deformations.

References:

[1] A. Düster, J. Parvizian, Z. Yang, and E. Rank, "The finite cell method for three-dimensional problems of solid mechanics", *Comput. Methods Appl. Mech. Eng.*, vol. 197, no. 45, pp. 3768-3782, Aug. 2008, https://doi.org/10.1016/j.cma.2008.02.036.
[2] W. Garhuom, S. Hubrich, L. Radtke, and A. Düster, "A remeshing strategy for large deformations in the finite cell method", *Comput. Math. Appl.*, vol. 80, no. 11, pp. 2379-2398, Dec. 2020, https://doi.org/10.1016/j.camwa.2020.03.020.

Incorporating knowledge of the material tangent for the data-driven discovery of hyperelastic material models

Nguyen, Duc Hoang *(Universität Augsburg, Germany)* 08:50
Weißenfels, Christian *(Universität Augsburg, Germany)*

The development of new complex materials inevitably leads to the request of new epistemic knowledge in materials modeling to optimize their benefits in terms of cost and performance during the virtual design phase. With the rise of modern experimental techniques and machine learning data-driven approaches for the extraction of epistemic knowledge in materials modeling are becoming more interesting.

We propose a new data-driven approach to discover the constitutive laws of isotropic hyperelastic materials. In contrast to black-box models like neural networks we obtain interpretable models by using sparse regression with a large library of candidate functions for the strain

density function. This approach only takes stress and strain data, which are directly available through experimental testing. Unlike other approaches we incorporate the material tangent in the optimization process by approximating the secants between data points. In order to obtain a parsimonious strain density function we promote sparsity through L1 regularization. This non-linear optimization problem is solved by a cyclic coordinate descent algorithm with backtracking line search. Due to the many non-linearities in the library of candidate functions all gradients and derivations are derived through automatic differentiation. The regularization term is selected via cross validation.

We show on several isotropic hyperelastic material models reflected in synthetic data - with and without noise - that our approach yields good results in terms of errors and convergences.

Experimental and numerical analysis of strain and thermal behaviour on 3D-printed flexible auxetic structures

Pi Savall, Berta *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Universität Stuttgart, Germany)*
Seyedpour, Seyed Morteza *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Universität Stuttgart, Germany)*
Tim, Ricken *(Institute of Structural Mechanics and Dynamics in Aerospace Engineering, Universität Stuttgart, Germany)*

09:10

The research focuses on the behaviour of a reentrant auxetic structure under uniaxial loading. The study uses a combination of experimental testing with a DIC system to measure the strain field and a thermal camera to record temperatures over time. Numerical simulation is developed to characterize the material response of the structures. The results of the study show that the 3D-printed flexible auxetic structures have unique mechanical properties that can be controlled by adjusting the design and material parameters. This research contributes to the understanding of the behaviour of flexible auxetic structures and can be used in a number of fields such as aerospace, energy storage, and biomedical engineering.

S04-03: Structural mechanics

Date: May 31, 2023 14:00-16:00
Room: HSZ/AUDI

Modular Topology Optimization Aided by Deep Learning

Gaynutdinova, Liya *(Czech Technical University in Prague, Czech Republic)* 14:00
Doškář, Martin *(Czech Technical University in Prague, Czech Republic)*
Rokoš, Ondřej *(Eindhoven University of Technology)*
Pultarová, Ivana *(Czech Technical University in Prague, Czech Republic)*
Hendriks, Fleur *(Eindhoven University of Technology)*

Optimization is a key aspect in the design of structures, mechanisms, and materials, as it allows for better performance, sustainability, and reduction of costs. However, the efficient use of resources encompasses the whole lifecycle of the design, thus the reusability and reparability must be considered. With these goals in mind, modular components that enable mass production and reconfigurability become highly desirable. The problem of modular designs is challenging because the module design problem is not convex and is strongly dependent on initial guesses. Heuristic methods like genetic algorithms (GA) are usually employed to address this issue, using the finite element analysis (FEA) for the objective function evaluation. FEA is computationally intensive, however, so the need for an efficient surrogate with adequate accuracy is apparent.

In this contribution, we consider the problem of optimizing a modular structure made up of modules of a limited number of types. Here ANN can provide a surrogate model but can be also incorporated into a solution process in a more sophisticated way (by providing derivatives, generating samples, etc.). We aim to build a sufficiently accurate and cheap surrogate model based on ANN as well as to define a strategy to use ANN in specific problems of modular design. An appropriate surrogate model can substantially speed up the heuristic optimization algorithms, as well as potentially bypass the iterative processes altogether if the approximation of the inverse mapping between the input parameters and the objective function is obtained.

Modified Settlement-Stability-Optimization Method for Numerical Foundation Design of Tower Cranes

Müllner, Herbert W. *(PORR Bau GmbH, Technology Management and Innovation, Vienna, Austria)* 14:20
Koza, Martin *(pde Integrale Planung GmbH, Structural Engineering, Premstätten, Austria)*

The static design of foundations for tower cranes is mostly based on calculations of structural safety like tilting, sliding and groundbreaking. Settlement calculations for evaluating the inclination of the crane, which is restricted by the suppliers of tower cranes [1], are essential for safe and economic foundation solutions, too. These calculations consider the interaction between soil and structure and allow asymmetrical foundation solutions. Furthermore, the influence on nearby temporary construction pit systems and slopes is clearly identified.

Thus, a method [2] has been developed satisfying the normative and crane specifically requirements and meeting the standards of one of the biggest building contractors in Europe. It is based on the conventional assumption that the crane exerts a quasi-constant load on the foundation. Therefore, the calculated settlements are too large. This lead to uneconomic foundation measurements for a majority of crane foundations.

This was one of the motivations for starting a research project in the field of numerical and experimental investigation of crane foundations. These investigations cover the analysis of the dead load of a crane construction and the corresponding wind force assumptions, the usage of geomechanical half-space analysis and combined stiff modulus method, respectively. Because the implementation of a generally valid calculation algorithm is not possible due to the large number of boundary conditions and the respective soil conditions on the specific construction site situation, the results of the research project were combined with the original method [2].

In this contribution the method and its application on various building sites in Austria is presented. In order to investigate whether the new calculation method is generally valid for future construction site applications, a successful validation of the new method is done by surveying the corner points of the corresponding foundation.

[1] C. Eiwan, M. Kraupatz: Erläuterungen und Hinweise zur Anwendung der statischen Daten der Betriebsanleitung von Liebherr Turmdrehkränen. LIEBHERR Werk Biberach GmbH Berechnungsmitteilung 0006 (2011).
[2] H.W. Müllner, H.R. Meister: Soil Mechanical Influence on Numerical Foundation Design of Tower Cranes; PAMM, 19 (2019), 1, https://doi.org/10.1002/pamm.201900119

Identification of creep parameters from multi-step relaxation tests on miniaturized specimen

Schirmer, Richard Wolfgang *(TU Bergakademie Freiberg, Germany)*
Selent, Marcel *(TU Bergakademie Freiberg, Germany)*
Abendroth, Martin *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*

14:40

The Small Punch Test (SPT) is a miniaturized method for thermo-mechanical materials testing. The combination of simple specimen geometry and low required specimen volume is ideal for minimally invasive characterization and monitoring of the current material condition in technological systems, including nuclear plants.

The aim of the present study is to identify creep material properties of the chromium steel P91 (X10CrMoVNb9-1) via Small Punch testing. It is examined to which extent a single relaxation test is suitable to replace several creep tests at different force levels. The inverse parameter identification method utilizes a non linear optimization approach in order to match the results of simulation and experiment. The simulation is performed using finite element analysis (FEA) and the considered material law aims to represent the high-temperature behavior of steels. To this end, the *Norton* creep law is specifically used along with linear elasticity and non linear isotropic plasticity. We propose a strategy, that can be used to separately identify the *Norton*-parameters from multi-step relaxation tests performed on one specimen. Thereby, the applied strain (displacement, if utilizing SPT) is kept constant after initial loading, which enables stress relaxation within the specimen. In case of the SPT, this behavior

yields a decreasing reaction force which approximately approaches a constant value. During the repeated loading phases, specimen failure may occur, due to further plastification of the specimen. Loading and relaxation cycles are repeated until specimen failure. These kinds of experiments are especially important for high-temperature bolting applications, where the clamping force decreases with time.

The identified parameters are validated via Small Punch creep experiments at different force levels. It will be shown that good agreement is observed when comparing the sets of identified parameters.

Multi-objective optimization in design and synthesis of compliant mechanisms

Humer, Alexander *(Johannes Kepler University Linz, Austria)*
Platzer, Sebastian *(Johannes Kepler University Linz, Austria)*
Pechstein, Astrid *(Johannes Kepler University Linz, Austria)*

15:00

"If something bends to do what it is meant to do, then it is compliant. If the flexibility that allows it to bend also helps it to accomplish something useful, then it is a compliant mechanism", is how Larry Howell describes the essence of compliant mechanisms. In contrast to conventional mechanisms, compliant mechanisms rely on flexible deformation, which is determined by their geometric shapes and material properties. Owing to the absence of relative sliding motion, compliant mechanisms allow us to eschew drawbacks typical of conventional mechanisms: Besides the reduction in parts, they show little friction, if any, and minimal wear. On the downside, design and synthesis of compliant mechanisms become much more involved than in rigid-body linkages—even more so as deformations involved become large and need to be distributed over flexible (sub-)structures to stay within the elastic range. Therefore, the analysis of compliant mechanisms requires both geometric and physical non-linearities to be accounted for. With finite stiffnesses being a defining property of compliant mechanisms, we face a trade-off between a maximum compliance regarding the intended motion and maximum stiffnesses in all orthogonal directions. Under dynamic actuation and loads, resonant frequencies of the mechanisms as a whole, but also internal resonances of sub-structures need to be considered in the synthesis. Optimization lies at the heart of any synthesis problem, irrespective of whether conventional rigid-body or compliant mechanisms are concerned. In compliant mechanisms we deal with multiple—typically conflicting—kinematic, static and dynamic objectives that do not admit globally optimal solutions but demand for compromises. By employing multi-objective optimization methods and their pivotal notion of Pareto-optimality, we avoid an a priori weighting among objectives, which inevitably introduces bias for certain designs. To efficiently explore the design space, we propose a hybrid two-stage approach for the synthesis of large-deformation mechanisms: Structural models provide effective means to capture the global behavior mechanisms in a first step. In a second step, continuum models allow us to resolve details and fine-tune design variants. We demonstrate the effectivity of the proposed approach by means of several representative examples ranging from elementary joints to complex mechanisms.

Theoretical aspects and applications of goal-oriented reanalysis methods

Materna, Daniel *(Ostwestfalen-Lippe University of Applied Sciences and Arts, Germany)* 15:20

In this contribution a method for goal-oriented reanalysis is presented. The method allows the prediction of the change in a quantity of interest due to structural modifications (design changes), e.g. the shape, the topology, material properties, etc. The approach is based on a goal-oriented method by using the primal and dual problems. Furthermore, the method is easily to implement in existing finite element programs, because no derivatives with respect to the design variables are necessary. The proposed method can be used in classical applications with successive design steps, for instance structural optimization, reliability analysis or structural damage analysis. In many cases hundreds or even thousands of different design configurations are investigated, and the state equation must be solved for each design step. The repeated structural analysis and the calculation of quantities of interest involves significant computational effort. Goal-oriented reanalysis methods can be used in order to reduce the overall computational cost in the numerical simulation.

A novel surrogate modelling approach for additive manufacturing processes

Hürkamp, André *(Technische Universität Braunschweig, Germany)*
Ekanayaka, Virama *(Technische Universität Braunschweig, Germany)* 15:40

Additive manufacturing (AM) enables the production of complex and customized components with minimal waste. However, to achieve the desired geometry and quality, a lot of process optimization is need (often by experimental trial and error). Especially, in the case of AM with concrete materials, the time dependent behaviour of the wet concrete is a large challenge to achieve process stability. Simulations taking into account the time dependent material are able to predict the printing result. However, these simulations are computationally intensive and require large computational resources. In order to speed up the process optimization before printing (offline) or even use simulations parallel to printing for process control (online) a sophisticated surrogate model is needed for the use in real-time manufacturing applications. To address this challenge, Proper Orthogonal Decomposition (POD) in combination with machine learning techniques has emerged as a promising surrogate modelling technique. In this contribution, a POD-based reduced order model for additive manufacturing is presented. Based on snapshots along the build-up process, a surrogate model is constructed that is able to predict the printing result with respect to the underlying process and materials. In combination with deep learning methods, such a procedure shows good agreement with full scale models for fixed geometries. In order to allow for a wider range of geometries, a novel surrogate modelling approach for AM inspired by POD is investigated using the initial waypoints of the printing trajectory as input. In this case, it is possible to analyse the manufacturing process for arbitrary geometries. The proposed method will be demonstrated for the use case of additive manufacturing with concrete materials.

S04-04: Structural mechanics

Date: June 1, 2023 08:30-10:30
Room: HSZ/AUDI

Locking-free coupling of continuum and shell elements in large deformation problems

Pechstein, Astrid *(Johannes Kepler University Linz, Austria)* 08:30
Neunteufel, Michael *(TU Vienna, Austria)*
Krommer, Michael *(Johannes Kepler University Linz, Austria)*

In many applications, thin shell-like structures are integrated within or attached to volumetric bodies. This includes reinforcements placed in soft matrix material in lightweight structure design, or hollow, filled structures. Finite element simulations of such setups are highly challenging. A brute force discretization of structural as well as volumetric parts using well-shaped three-dimensional elements may be accurate, but leads to problems of enormous computational complexity even for simple models. An alternative is the usage of shell elements for thin-walled parts. While these elements are designed such that locking is avoided even for small thicknesses, the coupling to nodal volumetric elements is not straightforward due to the different nature of degrees of freedom in shell and volume elements. Degrees of freedom of volume elements usually are defined through nodal displacements located at element nodes. For shells, classical shell theories include not only displacement or position of the center surface, but also the surface normal. Thus, differentiability of the shell surface is a prerogative, which is not met by standard volume elements. Coupling these different approaches is not straightforward, and may easily lead to severe locking if not done carefully. Neunteufel and Schöberl proposed a mixed shell element where, apart from displacements of the center surface, bending moments are used as independent unknowns. These elements were not only shown to be locking free and highly accurate in large-deformation regime, but also do not require differentiability of the shell surface. They can directly be coupled to classical volume elements of arbitrary order by sharing displacement degrees of freedom at the center surface. As the elements can be used on unstructured meshes, adaptive mesh refinement based on local stress and bending moments can be used. We present computational results that confirm exceptional accuracy for problems where thin-walled structures are embedded as reinforcements within soft matrix material.

Investigations on adapted interpolation orders for a displacement-strain-mixed isogeometric formulation

Stammen, Lisa *(BTU Cottbus-Senftenberg, Germany)* 09:10
Dornisch, Wolfgang *(BTU Cottbus-Senftenberg, Germany)*

Within isogeometric analysis, non-uniform rational B-splines (NURBS) are used for the discretization of the geometry as well as for the interpolation of the unknowns during the analysis. Hence, compared to standard finite element formulations, more accurate results can be obtained. Moreover, the continuity of the basis functions can be varied. Using mixed formulations, unknowns of several fields are interpolated independently. Therefore, differing basis functions are employed, whose continuities and degrees can be defined distinctly. While

mixed formulations can tackle certain locking effects, special issues concerning the stability of such formulations have to be considered. Furthermore, by selectively decreasing specific approximation orders, the computational effort can be reduced in comparison to standard formulations and consistency conditions can be ensured.

As the occurrence of non-coinciding basis function degrees in the strain-displacement formulation diminishes the exactness of results for standard formulations, a displacement-strain-mixed formulation with adapted interpolation orders is investigated in this contribution. Additionally, involving isogeometric analysis enables to study the potential of different combinations of continuities simultaneously. Thus, further investigations regarding the stability of mixed isogeometric formulations are conducted for various combinations of selected interpolation degrees and continuities. Furthermore, the convergence behavior and locking-resistance of the different variants of the investigated formulation is studied for a plane-stress benchmark problem for varying slenderness-ratios and compared to results of a standard non-mixed isogeometric formulation.

Accurate and efficient explicit structural dynamics via finite element technology-based selective mass scaling

Oesterle, Bastian *(Hamburg University of Technology, Germany)*
Hoffmann, Moritz *(Hamburg University of Technology, Germany)*
Tkachuk, Anton *(Karlstad University, Sweden)*
Bischoff, Manfred *(University of Stuttgart, Germany)*

09:30

The conditional stability of explicit algorithms for transient analyses limits the so-called critical time step size, which directly depends on the highest natural frequency of the discrete system. In case of shear deformable structural finite elements, for instance Reissner-Mindlin shell elements, the efficiency is limited by the highest transverse shear frequencies. When thin-walled structures are discretized by solid or solid shell elements, the critical time step is limited by the highest frequencies associated with thickness stretch of the elements [1]. In most cases, the highest frequencies have a minor influence on the overall structural response but severely decrease the efficiency of explicit schemes.

The aim of selective mass scaling (SMS) is to scale down the highest frequencies in order to increase the critical time step size, while keeping the important low frequency modes as unaffected as possible. SMS concepts are designed such that at least translational inertia is preserved [2], whereas the preservation of rotational inertia mostly comes along with high additional computational costs.

In this contribution, we present recent investigations on a novel class of SMS techniques, which are based on a concept from finite element technology, that is the Discrete Strain Gap method [3]. Similarities and opposites to the recently introduced concept of intrinsically selective mass scaling [4] are discussed for the case of shear deformable structural element formulations. Furthermore, extensions of the novel SMS techniques to solid and solid shell elements are presented, which preserve both translational and rotational inertia. The novel SMS concepts are compared to existing ones with respect to efficiency, accuracy, generality and robustness.

[1] G. Cocchetti, M. Pagani und U. Perego. Selective mass scaling and critical time-step estimate for explicit dynamics analyses with solid-shell elements. *Computers & Structures,* Vol.**127**, pp. 39-52, 2013.
[2] L. Olovsson, K. Simonsson und M. Unosson. Selective mass scaling for explicit finite element analyses. *Int. J. Numer. Meth. Engng.,* Vol. **63(10)**, pp. 1436-1445. 2005.
[3] K.-U. Bletzinger, M. Bischoff und E. Ramm, A unified approach for shear-locking-free triangular and rectangular shell finite elements. *Computers & Structures*, Vol. **75(3)**, pp. 321-334. 2000.
[4] B. Oesterle, J. Trippmacher, A. Tkachuk and M. Bischoff, Intrinsically Selective Mass Scaling with Hierarchic Structural Element Formulations. Book of Extended Abstracts of the 6th ECCOMAS Young Investigators Conference 7th-9th July 2021, Valencia, Spain, 2021.

A Highly Efficient Lagrange Multiplier Based Mixed Finite Element Formulation for Gradient Damage

Riesselmann, Johannes *(Ruhr University Bochum, Germany)* 09:50
Balzani, Daniel *(Ruhr University Bochum, Germany)*

Local damage formulations are challenged with mesh-dependency and the loss of ellipticity at already moderate damage states. Through gradient enhancement, the damage solution field of corresponding formulations posesses a higher regularity leading to mesh-independent solutions and an increased numerical robustness. In this contribution, a corresponding Lagrange multiplier based mixed finite element formulation for finite strains is presented. A suitable FE-interpolation scheme allowing for computational cost reduction through static condensation is introduced. A simple update scheme for modeling the evolution of the damage variable is presented allowing for a straightforward implementation using classical user element interfaces. In numerical tests, mesh-independent solutions, robustness of the solution procedure for states of severe damage and under cyclic loading conditions are presented. Furthermore, an improved convergence behavior compared to the penalty approach is shown.

Geometrically Nonlinear Locking Phenomena that are Unknown from Linear Analysis

Bieber, Simon *(Universität Stuttgart, Germany)* 10:10
Willmann, Tobias *(Universität Stuttgart, Germany)*
Bischoff, Manfred *(Universität Stuttgart, Germany)*

The issue of locking in solid and structural finite elements is known since decades. Until today, development of locking-free finite element formulations is an active field of research. Numerous remedies have been developed and locking-free formulations are available for many linear and non-linear applications Interestingly, scientific studies on the origins of different locking phenomena, such as shear locking and volumetric locking, which are an indispensable prerequisite for development of locking-free methods, almost exclusively focus on linear analyses. The corresponding formulations are then straightforwardly extended to the geometrically and materially non-linear case. A careful study of locking for geometrically nonlinear analysis, however, reveals that there are distinct nonlinear locking phenomena, not

previously described in the literature. These are not remedied by the standard methods to avoid locking.

This contribution highlights the existence of nonlinear locking effects that exclusively show up in the presence of large deformations. These effects may significantly deteriorate the accuracy of finite element solutions, especially for thin-walled structures and nearly incompressible material behavior. We provide a systematic analysis of these rarely known phenomena and show that classical unlocking schemes are not sufficient to avoid them. The issue is discussed in detail for the Enhanced Assumed Strain (EAS) method, which is frequently used to avoid volumetric locking and shear locking in solid elements. Finally, strategies to avoid nonlinear locking phenomena are presented.

S04-05: Structural mechanics

Date: June 1, 2023 16:00-19:00
Room: HSZ/AUDI

Multidomain physics-informed neural networks for analysis of 2D thin-walled structures

Zhang, Peijun *(University of Siegen, Germany)* 16:00
Gu, Yan *(University of Siegen, Germany)*
Zhang, Chuanzeng *(University of Siegen, Germany)*

Thin-walled composites are widely used in many fields of science and engineering. Numerical simulation of such structures has long been a computational challenge. Due to the special geometric configuration of thin-walled composite structures, where the thickness-to-length ratio is extremely small, standard numerical methods are difficult to apply to such structures. In this work, we present a method to handle such thin-walled using multi-domain physics-informed neural networks (MPINNs) optimized to satisfy the governing partial differential equations and the corresponding boundary conditions. The present PINNs-based method is meshless, which is a key feature as the conventional mesh-based methods become computationally expensive for ultrathin-walled composite structures. Furthermore, the present method based on MPINNs decomposes the thin-walled composite structures into sublayers and uses proper interface constraints to couple them together. Numerical examples will be presented and discussed to show the accuracy and efficiency of the present MPINNs-based method.

Full-field prediction and target design of nonlinear metamaterial responses via probabilistic models

Bastek, Jan-Hendrik *(ETH Zürich, Switzerland)* 16:20
Kochmann, Dennis M. *(ETH Zürich, Switzerland)*

The accelerated inverse design of nonlinear material properties, i.e., identifying a material with a given stress-strain response over a finite deformation path, holds great potential for addressing pressing challenges in, e.g., soft robotics, biomedical implants, and energy absorption. Machine learning models have received significant attention and demonstrated success in obtaining such highly nonlinear mappings, though they have typically been applied to linear properties, such as the directional Young's modulus, and rarely to more complex settings as the ones mentioned above [1]. We here address this challenge and present a novel framework that leverages recent advances in generative deep learning models. Specifically, we develop a diffusion model [2] trained on the full-field data of periodic stochastic structures obtained via finite-element (FE) simulations to predict the deformation and stress response of these structures in the finite-strain regime. By conditioning the model on a target stress-strain response, it generates a large variety of structures that closely match the desired curve for compressive strains of up to 20%. Unlike commonly encountered black-box models, our framework intrinsically provides a complete full-field estimate of the expected deformation path, including the internal stresses which closely align with results obtained via simulations.

This eliminates the need for a complex setup of FE frameworks to verify the designed structures and their stress-strain responses. This work has thus the potential to greatly simplify and accelerate the identification of materials with complex target properties.

[1] Deng, B., Zareei, A., Ding, X., Weaver, J. C., Rycroft, C. H., & Bertoldi, K. (2022). Inverse Design of Mechanical Metamaterials with Target Nonlinear Response via a Neural Accelerated Evolution Strategy. *Advanced Materials*, 34(41). https://doi.org/10.1002/adma.202206238.
[2] Ho, J., Jain, A., Abbeel, P. (2020). Denoising Diffusion Probabilistic Models. https://arxiv.org/abs/2006.11239.

Generative learning based model for the prediction of 2D Stress distribution

Gulakala, Rutwik *(Institute of General Mechanics (IAM), RWTH Aachen University, Germany)*
Markert, Bernd *(Institute of General Mechanics (IAM), RWTH Aachen University, Germany)*
Stoffel, Marcus *(Institute of General Mechanics (IAM), RWTH Aachen University, Germany)*

16:40

Machine learning-based algorithms are gaining a lot of momentum for accelerating the computation time of structural simulations. Deep learning methods have demonstrated excellent results when utilized to speed up the physical simulations and learn the underlying physics without prior knowledge of the mechanical model [1]. The aim of the study is to explore the ability of a Generative learning-based approach in predicting the output of Finite Element simulations. Often, the drawback of classical regression models is that they are bound to the distribution of training data and cannot extrapolate outside of the training domain. In the current study, to overcome this, we propose a GAN-based approach for learning to infer structural mechanics simulations. GANs have the ability to learn the underlying distribution of data and can efficiently extrapolate outside the training range. They have already proven to be an extremely capable and powerful tool in natural language processing and generating non-existing, realistic synthetic data from a given input condition [2, 3]. We train the proposed network on data obtained from classical Finite Element simulations based on linear elastic, Johnson-Cook plasticity [4] and Lemaitre-Chaboche viscoplastic models [5]. The goal here is to understand the ability of a GAN to replace FEM by incorporating the underlying mechanics knowledge into the network to enhance the generalizing ability of the network for various materials on various loading and boundary conditions.

[1] M. Stoffel, R. Gulakala, F. Bamer and B. Markert, “Artificial neural networks in structural dynamics: A new modular radial basis function approach vs. convolutional and feedforward topologies,” *Computer Methods in Applied Mechanics and Engineering,* no. 364, p. 112989, 2020.
[2] R. Gulakala, B. Markert and M. Stoffel, “Rapid diagnosis of Covid-19 infections by a progressively growing GAN and CNN optimisation,” *Computer Methods and Programs in Biomedicine,* vol. 229, no. 1, 2022.
[3] T. Brown, B. Mann, N. Ryder, M. Subbiah, J. D. Kaplan, P. Dhariwal and A. Neelakantan, “Language models are few-shot learners.,” *Advances in neural information processing systems 33,* pp. 1877-1901, 2020.
[4] G. R. Johnson and W. H. Cook, “A Constitutive Model and Data for Metals Subjected to Large

Strains, High Strain Rates, and High Temperatures," in *Proceedings 7th International Symposium on Ballistics*, The Hague, 1983.
[5] J. Lemaitre and J.-L. Chaboche, Mechanics of solid materials, Cambridge university press, 1994.

Modelling of additive manufacturing processes with time-dependent material properties using physics-informed neural networks

Ekanayaka, Virama *(Technische Universität Braunschweig, Germany)* 17:00
Hürkamp, André *(Technische Universität Braunschweig, Germany)*

Physics informed neural networks (PINN) have recently gained a lot of popularity due to their effectiveness in solving differential equations utilizing artificial neural networks. The effectiveness of this method is the absence of a traditional labelled data set, where instead so-called collocation points from the input space of the differential equation are used. The minimized loss function includes the differential equation computed at the collocation points as well as the summation of all boundary conditions. It has been shown that PINNs can be implemented to tackle different problems in solid mechanics and for the theory of elasticity. In the existing literature, the governing differential equations for static structural problems have been solved, where the deformation can then be predicted for constant material properties. This paper provides an extension of this approach to include time-dependant material properties when solving the governing differential equations in order to model the additive manufacturing process with time-dependent material properties. The PINN is then generalized and capable of solving problems in structural mechanics with varying material properties and is not anymore component or material specific. The effectiveness of the method is then verified by comparing its results with a finite element simulation for a component with time-dependent material properties.

Effects of Variational Formulations on Physics-Informed Neural Network Performance in Solid Mechanics

Radin, Nils *(Chair of Structural Analysis and Dynamics, RWTH Aachen University, Mies-van-der-Rohe-Str.1, 52074 Aachen, Germany)* 17:20
Klinkel, Sven *(Chair of Structural Analysis and Dynamics, RWTH Aachen University, Mies-van-der-Rohe-Str.1, 52074 Aachen, Germany)*
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In recent years, physics-informed neural networks (PINNs) have emerged as a promising method for solving partial differential equations (PDEs) in a variety of fields. To this end, an artificial neural network is used to approximate the unknown variables while the differential equation is embedded in the loss function to penalize the network's output. The present contribution focuses on the application of PINNs in the field of solid mechanics. We formulate and develop the PINN framework by incorporating the strong form of the PDE alongside initial and boundary conditions into the loss function of the neural network. The loss function poses as a residual, effectively constructing a minimization problem to solve the PDE. The nature of the residual is further reformulated into the variational (weak) form by applying

test functions and integration by parts. This extension leads to variational physics-informed neural networks (VPINNs), which impose a lower stringency on the solution. We demonstrate the performance of both PINNs and VPINNs on numerical benchmark problems, such as the square plate with a circular hole. Specifically, the relaxed requirements on the solution imposed by VPINNs prove to reduce training cost while simultaneously increasing accuracy and stability. PINNs employing the strong form demonstrate advantages in applying boundary conditions to truncated domains.

A Label Machine for Mechanical Systems: Discovering Operating States with Unsupervised Learning from load time series

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Hantschke, Peter *(Technische Universitat Dresden, Institute of Solid Mechanics, 01062 Dresden, Germany)*
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17:40

Accurate labeling of the operating states of mechanical systems is a fundamental aspect of analyzing their usage profiles. Manual labeling of states is typically time consuming and requires expert knowledge of the system, making it impractical for large datasets. In recent years, unsupervised learning techniques have emerged as a promising alternative to automate the identification of operating states for mechanical systems.

In this work, we propose an automated approach for identifying operating states of mechanical systems using a scattering transform for extracting a time-frequency representation from load time series. To label the states, we apply a principal component analysis and a Gaussian mixture model clustering. The proposal includes separating the hyperparameters of the algorithm into a parameter-set that needs to be defined through minimized expert knowledge in comparison to manual labeling. All remaining hyperparameters can be determined automatically through standard hyperparameter optimization techniques (e.g. grid search).

To evaluate our approach, we conduct experiments on real-world datasets and compare the discovered operating states with those generated through expert knowledge. The results demonstrate the effectiveness of the concept and show that it can provide a promising alternative to manual state labeling.

Effective mechanical properties of architectured materials: forward prediction and inverse design by data-driven methods

Peng, Xiang-Long *(Division Mechanics of Functional Materials, Institute of Materials Science, TU Darmstadt)*
Xu, Bai-Xiang *(Division Mechanics of Functional Materials, Institute of Materials Science, TU Darmstadt)*
18:00

Like other microstructured materials, effective properties of beam-based architectured materials strongly depend on their underlying microstructures. This provides the opportunity to achieve on-demand effective properties by tailoring their microstructural features. To this end, both forward prediction and inverse design should be handled. The former predicts

the effective properties of a specified microstructure, which can be readily done by analytical approaches in few cases and more generally by computational homogenization. The latter provides a microstructure design with target effective properties, which is a challenging task.

In this work, we consider the forward prediction and inverse design of the effective elastic properties of a number of typical beam-based periodic architectured materials based on data-driven methods. The effective elastic properties of these materials such as Young's modulus, Poisson ratio, and degree of anisotropy can span over a wide range by tuning the microstructural geometry. Thus, they have the potential to act as structural components in novel engineering systems where a large range of mechanical properties are desired.

Firstly, we generate a dataset consisting of microstructural parameters paired with the corresponding effective properties. For this purpose, we create a large number of unit cell designs with various microstructural parameters such as the strut thickness, inclined angle and aspect ratio for each individual structure. Their effective properties will be evaluated by computational homogenization. Then, a forward neural network surrogate model for forward prediction is trained by the dataset. Subsequently, a backward neural network for inverse design is trained by the same dataset, where the effective properties and microstructural parameters are respectively the inputs and outputs. To tackle the issue that multiple structures may yield the same effective properties, a loss function quantifying the difference between the target (input) properties and those of the designed (output) structure evaluated by the forward model is adopted. Eventually, the two trained neural network models enable the forward prediction and inverse design of the effective elastic properties of the considered architecture materials without any further simulation efforts, which facilitates their application in practice. The proposed methodology can be adapted to investigate other microstructured materials in terms of mechanical as well as functional properties.

On the role of locking in solving structural mechanics problems via physics informed neural networks

Striefler, Lukas *(Hamburg University of Technology, Germany)* 18:20
Oesterle, Bastian *(Hamburg University of Technology, Germany)*

In recent years, artificial intelligence (AI) has gained widespread attention due to breakthrough research progress and a number of practical applications in our daily life. Also, numerous branches of applied mathematics and computational mechanics try to exploit the potential of AI, in particular artificial neural networks (ANNs). By incorporating laws of physics into ANNs, so-called physics informed neural networks (PINNs) [1] eliminate the need for extensive training data. Most of the proposed PINN frameworks for structural mechanics applications incorporate information about the partial differential equations (PDEs) in the loss function via energy methods [2] or collocation methods [3].

For typical problems in structural mechanics, the underlying PDEs are stiff, resulting in well-known locking effects, already recognized in the early days of finite element analysis. But locking effects are present for all discretization schemes, not only for finite elements, independent of the polynomial order, smoothness, or any other criterion. This is true for both Galerkin-type solution methods and for collocation methods based on the Euler-Lagrange equations of the specific boundary value problem [4].

In this contribution, we study the role stiff PDEs or locking effects on the accuracy and efficiency of PINN-based numerical solutions of problems in structural mechanics. We present first investigations on the use of PINNs for solving shear deformable beam and plate problems. Different types of beam and plate formulations, as well as different types of collocation-based loss functions are evaluated and compared with respect to accuracy and efficiency.

[1] M. Raissi, P. Perdikaris, G.E. Karniadakis. Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. *Journal of Computational Physics*, Vol. **378**, pp. 686-707. 2019
[2] E. Samaniego, C. Anitescu, S. Goswami, V.M. Nguyen-Thanh, H. Guo, K. Hamdia, X. Zhuang, T. Rabczuk. An energy approach to the solution of partial differential equations in computational mechanics via machine learning: Concepts, implementation and applications. *Computer Methods in Applied Mechanics and Engineering*, Vol. **362**, 112790. 2020
[3] H. Guo, X. Zhuang, T. Rabczuk. A Deep Collocation Method for the Bending Analysis of Kirchhoff Plate. *Computers Materials & Continua*. Vol. **59(2)**, pp. 433-456. 2019
[4] B. Oesterle, S. Bieber, R. Sachse, E. Ramm, M. Bischoff. Intrinsically locking-free formulations for isogeometric beam, plate and shell analysis. *Proc. Appl. Math. Mech. 2018*, **18**:e20-180039. 2018

Using Conditional Generative Adversarial Networks for the Prediction of Stresses in a Adhesive Composite

Khan, Abdul Wasay *(Institut für Windenergiesysteme, Leibniz Universität Hannover)* 18:40

Fibre reinforced adhesives are an integral part of wind energy turbine blades and play an important role in evaluation of structural integrity of the blades. Digitization of manufacturing processes and demand for fast and efficient stress analysis argues for the application of deep learning. As a step forward in using deep learning to predict structural properties in composite, the work would explore the applicability of deep learning methods to 2D fibre reinforced composite. In this work, a composite adhesive used in wind energy turbine blades is used as an illustrative example. The composite adhesive when viewed using a CT scanner shows a heterogeneous structure with two phases, a softer matrix phase and a more stiff fibre phase. For this purpose, several CT scan images of the fibre adhesive composite are used. Also, a strategy to generate representative images for the CT Scan images is sought using generative adversarial networks for the general applicability of the method. The images on subsequent FEA analysis serves as the training data for the deep learning framework. Once trained, the neural network would be able to predict the stress distributions in the structure. We apply conditional adversarial networks as a general purpose solutions to stress prediction problem which be thought of as image-to-image translation problems. These networks in addition to learning the mapping from input image to output image also learn a loss function to train for this mapping. This makes the method more generic because otherwise different loss formulations for different problems have to be formulated. Inspiration is also sought from semi semantic segmentation problems where training deep networks with limited labeled data while attaining a strong generalization ability is necessary in the goal to cut human annotation efforts.

S04-06: Structural mechanics

Date: June 2, 2023 08:30-10:30
Room: HSZ/AUDI

Comparison of modelling approaches for the bending behaviour of fibre-reinforced thermoplastics in finite element forming analyses

Kabala, Philipp *(Institut für Werkzeugmaschinen und Fertigungstechnik (IWF), Technische Universität Braunschweig, Germany)* 08:30
Middelhoff, Jan *(Institut für Werkzeugmaschinen und Fertigungstechnik (IWF), Technische Universität Braunschweig, Germany)*
Voigt, Dominik *(Institut für Werkzeugmaschinen und Fertigungstechnik (IWF), Technische Universität Braunschweig, Germany)*
Dröder, Klaus *(Institut für Werkzeugmaschinen und Fertigungstechnik (IWF), Technische Universität Braunschweig, Germany)*
Hürkamp, André *(Institut für Werkzeugmaschinen und Fertigungstechnik (IWF), Technische Universität Braunschweig, Germany)*

Fibre-reinforced thermoplastic (FRTP) composites are increasingly being used for structural applications as these offer short cycle times and good recyclability in addition to high specific strength and stiffness. For the production of shell like structural components, laminates made of unidirectional fibre tapes or woven fabrics (organo sheets) are draped in a thermoforming process. Due to the melted thermoplastic matrix, the composite exhibits a highly flexible (limp) behaviour during the forming process. Along with the intralaminar shear, bending is an essential mechanism in the forming process, influencing manufacturing-related defects like formation of wrinkles.

Especially the modelling of the proper bending behaviour during forming is a current challenge in the finite element analysis of thermoforming processes. In recent research, various approaches to model the bending behaviour of composites have been investigated to improve the numerical prediction accuracy of the forming behaviour.

In this contribution different modelling approaches for the temperature-dependent bending behaviour of FRTPs during forming are investigated and compared. For this purpose, the bending of uni-directional laminates and organo sheets is determined experimentally using cantilever beam tests. Based on the experimental data, the modelling approaches combining shell and membrane elements are calibrated and evaluated in forming simulations using LS-Dyna. Finally, a multi-criteria evaluation of the approaches is carried out.

Construction, modeling, and control of a three-beam prototype using interactive fiber rubber composites

Acevedo Velazquez, Aline Iobana *(TU Dresden, Faculty of Electrical and Computer Engineering, Institute of Control Theory (RST), Dresden, Germany)* 08:50

Keshtkar, Najmeh *(TU Dresden, Faculty of Electrical and Computer Engineering, Institute of Control Theory (RST), Dresden, Germany)*
Mersch, Johannes *(TU Dresden, Faculty of Electrical and Computer Engineering, Institute of Solid State Electronics (IFE), Dresden, Germany)*
Katzer, Konrad *(TU Dresden, Faculty of Mechanical Science and Engineering, Institute of Materials Science (IfWW), Chair of Materials Mechanics and Defect Analysis, Dresden, Germany)*
Röbenack, Klaus *(TU Dresden, Faculty of Electrical and Computer Engineering, Institute of Control Theory (RST), Dresden, Germany)*
Cherif, Chokri *(TU Dresden, Faculy of Mechanical Science and Engineering, Institute of Textile Machinery and High Performance Material Technology (ITM), Dresden, Germany)*
Gerlach, Gerald *(TU Dresden, Faculty of Electrical and Computer Engineering, Institute of Solid State Electronics (IFE), Dresden, Germany)*
Zimmermann, Martina *(TU Dresden, Faculty of Mechanical Science and Engineering, Institute of Materials Science (IfWW), Chair of Materials Mechanics and Defect Analysis, Dresden, Germany)*

The integration of sensors, actuators, and control circuit elements into soft structures gives rise to the so-called interactive composites. In particular, interactive fiber rubber composites (I-FRC) are a promising option for fields such as human-machine interaction and robotics. In this work, a prototype of interactive fiber rubber composite is designed and manufactured, with a structure that consists of three beams integrated with actuators that allow the control of spatial deformations. We used shape memory alloys (SMA) as actuators, these are integrated into a textile layer and covered with an elastomer layer that gives flexibility and protection. When we apply a voltage to the terminals of the SMAs, the temperature of the SMAs increases and produces a deformation, this prototype showed considerable deformation performing vertical movements but its performance doing lateral movements are negligible. Therefore, the model and control are only focused on the vertical movement when the three beams are activated. We developed a mathematical model that describes the behavior of the prototype using system identification. To obtain the parameters of the model we performed open-loop tests, such as applying different steps of voltage to the terminals of the SMAs, meanwhile we measure the deflection of the prototype during the heating and cooling process. Considering the voltage as input and the deflection as output, the measurements are used to do the parameter identification of the model, which can be represented as a first-order transfer function. Through this model, the characteristics of the prototype over a wide range of operating points were described. Due to the hysteretic behavior of SMAs and their inherent nonlinearities, precise position control of systems actuated by these materials is a challenging task. We have proposed a control technique that ensures robust, fast, and precise position tracking. Where different uncertainty models are included to compensate for the nonlinearities of the system, afterward a Proportional-Integral (PI) controller is designed

using these robust stability conditions, and we validate it with numerical simulations and real experiments.

Development of a finite element model for the simulation of the flexural behavior of pressed paper-based sandwich panels with a sinusoidal core

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Hirsch, Franz *(Institute for Solid Mechanics, TU Dresden, 01062 Dresden, Germany)*
Süße, Dietmar *(Institute for Solid Mechanics, TU Dresden, 01062 Dresden, Germany)*
Lutsch, Birgit *(Papiertechnische Stiftung, 01809 Heidenau, Germany)*
Kästner, Markus *(Institute for Solid Mechanics, TU Dresden, 01062 Dresden, Germany)*

09:10

Using sandwich structures with a sinusoidal core has contributed significantly to implementing paper-based lightweight structures in the automotive industry, thus promoting economic and sustainable mobility. The sandwich structure studied here is formed through a pressing process and is commonly used in automotive construction, such as car roofs in Jeep New Renegade. Therefore, the flexural strength and modulus of paper-based lightweight components are critical factors in the design of vehicles and equipment. The correlation between the flexural strength, manufacturing method, and layer compositions of pressed panels is investigated experimentally and numerically using three-point bending tests and corresponding finite element models.

The proposed finite element model for studying the flexural behavior of the pressed sandwich panel consists of a top layer, an intermediate layer, a corrugated core, and a bottom layer. The top layer is made of a high-gloss polymer material and is modeled as an isotropic elastic-plastic material. The remaining layers are machine-made paper materials, which exhibit orthotropic elastic-plastic behavior and are characterized by three principal material directions. The material properties for all layers were determined experimentally by tensile tests.

The pressing process was performed under various manufacturing conditions and with different intermediate materials. The panels are first compressed to selected heights by hot pressing to achieve the desired shape. After cooling to room temperature, the pressed panels are subjected to the three-point bending (TPB) tests. The experimental results of TPB are analyzed to estimate the influence of different manufacturing methods and materials on flexural strength. Afterward, numerical simulations using the commercial software Abaqus with an explicit solver for the quasi-static process are conducted based on the same process conditions. Finally, the simulation results are compared with the experimental data to evaluate the accuracy and reliability of the numerical model.

Approximate postbuckling analysis of shear deformable laminates

Schilling, Jakob Christian *(Technical University of Darmstadt, Department of Mechanical Engineering, Institute for Lightweight Construction and Design, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany)*
Mittelstedt, Christian *(Technical University of Darmstadt, Department of Mechanical Engineering, Institute for Lightweight Construction and Design, Otto-Berndt-Str. 2, 64287 Darmstadt, Germany)*

09:30

In the lightweight design of aircraft, spacecraft and marine vessels, often advanced materials are utilized. Advanced materials such as laminated composites made of fibre-reinforced plastics show transverse shear deformation if they are considered “thick” or possess little transverse shear stiffness. In most cases the effect of the shear deformation is neglected, and few computational models exist that consider the closed-form approximate analysis of the postbuckling behaviour. Thus, a new computational model based on high order shear deformation theories is introduced. The solution is derived based on the principle of the minimum of the total elastic potential and is evaluated in comparison to finite element analyses. The highly efficient approximate computational model is developed to offer a valuable tool for the preliminary design of lightweight structures utilising shear deformable advanced materials.

Thermal and mechanical characterization of PA6 with a focus on simulating thermoforming process

Kulkarni, Sameer Ravindra *(University of the Bundeswehr Munich, Germany)*
Lion, Alexander *(University of the Bundeswehr Munich, Germany)*
Johlitz, Michael *(University of the Bundeswehr Munich, Germany)*
Loos, Klara *(University of the Bundeswehr Munich, Germany)*
Reuvers, Marie-Christine *(RWTH Aachen University, Germany)*
Brepols, Tim *(RWTH Aachen University, Germany)*
Reese, Stefanie *(RWTH Aachen University, Germany)*

09:50

The ongoing research project focuses on developing a novel thermo-mechanically coupled constitutive model of a composite made of semicrystalline thermoplastic matrix and continuous glass fibers, with the ultimate aim of correctly simulating the thermoforming process. In the scope of this contribution, the focus is on modeling the crystallization kinetics in the matrix material PA6 and, secondly, on characterizing the crystallinity-dependent thermoviscoelastic properties of PA6. The objectives of crystallization kinetics modeling in this project are to identify the phase transition from melt to solid state, to consider the exothermic latent heat during crystallization in the thermal part of the analysis, and to determine the nonhomogeneous crystallinity distribution in the laminate resulting from uneven cooling in the thickness direction. Depending on the degree of crystallinity, the material’s mechanical properties in the solid state tend to vary significantly; hence a comprehensive study of the influence of the degree of crystallinity on the mechanical properties is necessary.

To model the crystallization kinetics, a modified form of the Avrami model, known as the Nakamura-Ziabicki model, is adopted. The parameters for the Nakamura-Ziabicki model, which depend on the cooling rate, are identified based on fitting the model to the Flash DSC and standard DSC non-isothermal cooling experiments. Finally, the model is implemented in

commercial FE software COMSOL, and crystallinity evolution in laminate is simulated for the process-relevant mold and laminate temperatures.

To account for the strain rate dependency in the material, hyper-viscoelastic modeling approach is used. The equilibrium part is modeled using Neo-Hooke's model, whereas generalized Maxwell model is used for the rate dependent part. Owing to the finite deformations observed during thermoforming, viscoelastic behavior is modeled in the framework of the multiplicative decomposition of the deformation gradient. Moreover, to determine the high strain rate response of the material, which is not readily available from the tensile machine, the concept of time-temperature superposition is utilized to generate a master curve based on relaxation results at different temperatures. The best-fit parameters of the model are then obtained by fitting to the master curve using the iterative inverse FE method.

Geometrically accurate one-point integration of higher order virtual elements in finite deformations

Bode, Tobias *(Institute of Continuum Mechanics, Leibniz University Hannover, Garbsen, Germany; Cluster of Excellence PhoenixD, Lebiniz University Hannover, Hannover, Germany)* 10:10

Modeling for the description and prediction of processes in nature often leads to partial differential equations. Solving these field equations can only be done analytically in very few cases, so that in practice numerical approximation methods are often used. Variational methods like the Galerkin method have proven to be very effective and are widely used in industry and research. To set up the system of equations, integration over the area to be calculated is necessary. For more complex geometries or nonlinear equations, analytical integration becomes difficult or even infeasible, so that integration is also often performed numerically in the form of weighted evaluations of the integrand, the Gauss quadrature. In order to benefit from the quasi-optimal accuracy of the Galerkin method according to Cea's lemma in the linear case, the quadrature scheme must also be of sufficient accuracy. On the contrary, for more complex constitutive laws, under-integration is often used in engineering to save computational time. Based on a split of geometric and material nonlinearities, the present talk introduces a one-point integration scheme that is able to integrate polynomial shape functions of arbitrary order geometrically accurately. The material nonlinearity can be captured with the desired accuracy via a Taylor series expansion from the nonlinear state. As a demonstration the integration scheme is applied to two-dimensional polygonal shaped second order virtual elements where the quadratic projection is integrated via a single integration point.

S04-07: Structural mechanics

Date: June 2, 2023 08:30-10:30
Room: HSZ/201

Inelastic and multiphysics beam modelling and simulation with isogeometric collocation methods

Alzate Cobo, Juan Camilo *(Technische Universität Darmstadt, Germany)* 08:30
Weeger, Oliver *(Technische Universität Darmstadt, Germany)*

The rise of additive manufacturing in recent years paves the way for the commercial fabrication of slender structures with tailorable mechanical properties. Such structures, e.g. lattices composed of beam elements, have a wide range of applications in the automotive industry, aeronautics, aerospace, biomedicine, etc. Nevertheless, the modeling and simulation of lattice structures with commonly used methods, such as continuum finite elements, is computationally expensive. A way to mitigate this adversity is the use of beam theories. They impose physically reasonable kinematic constraints on the beam's cross-section, thus projecting the deformation and load quantities of the structure to cross-sectional average values and therefore reducing the overall numerical effort. Another advantage of beam theories is the implementation of B-splines, or in general of NURBS, for the discretization of the beam's centerline and cross-sectional orientation. NURBS based discretization leads not only to a precise description of the beam's deformation, but it allows the use of the strong form equations of the linear and angular momenta of the beam. For the Cosserat beam theory, also referred to in the literature as the Timoshenko beam, a mixed isogeometric collocation method that alleviates shear locking phenomena has already been developed and validated for a linear elastic material model with small strains. Since the interest in modeling lattice structures goes beyond beams with linear elastic material models with small strains, there is also motivation in the development of plasticity and multiphysics models suited for Cosserat beams. For this reason, an extension of the mixed isogeometric collocation method towards inelastic material behaviors has recently been proposed. In this work, the model is further enhanced to simulate axial strains resulting from a temperature or a concentration field, i.e., one-dimensional diffusion processes are incorporated. Consequently, the present model represents the starting point for the coupling between thermodynamics, beam theory and isogeometric analysis. Furthermore, the development of a plasticity model suited for beam theory, comprised of a yield condition, a flow rule and a hardening rule exposes some difficulties. To this regard, the current limitations for the development of suitable plasticity models are discussed.

Isogeometric cohesive zone modeling of interfaces in reinforced concrete structures

Klinkel, Sven *(RWTH Aachen Universtity, Germany)*
Kikis, Georgia *(RWTH Aachen Universtity, Germany)*
Klarmann, Simon *(RWTH Aachen Universtity, Germany)*
Chudoba, Rostislav *(RWTH Aachen Universtity, Germany)*

08:50

In reinforced concrete structures, the correct representation of the bond between concrete and reinforcement is a challenging task, since different mechanisms are acting simultaneously. On the other hand, the exact description of the reinforcement's geometry is not sufficient when using Lagrange shape functions and can additionally alter the modelling of this interaction. Isogeometric analysis enables the exact representation of complex geometries, and thus, can improve the correct description of the interface mechanisms. The concrete matrix as well as the reinforcement are modeled using boundary representation together with NURBS and B-splines (SBIGA) which is in accordance with the modeling technique in CAD tools. This allows for a straightforward use of the design model in the analysis process. The interaction mechanisms between reinforcement and concrete are modelled using a zero-thickness interface in combination with a thermodynamically consistent cohesive zone model that captures the decohesion, compression and sliding effects. It includes a coupled damage-plasticity dissipation for the normal and tangential direction. The model is verified using experimental results and a comparison to the standard Finite Element Method is carried out in order to investigate the benefits of applying isogeometric analysis for the exact representation of the reinforcement.

An augmented stress resultant plasticity model to accelerate shell finite element simulations of sheet metal roll forming

Kocbay, Emin *(Institute of Mechanics and Mechatronics, TU Wien, Austria)*
Scheidl, Jakob *(Institute of Mechanics and Mechatronics, TU Wien, Austria)*
Vetyukov, Yury *(Institute of Mechanics and Mechatronics, TU Wien, Austria)*

09:10

In roll forming an initially flat metal sheet sustains incremental plastic bending as it passes through a series of roll stands. The final cross section shape is obtained by irreversible plastic bending deformation, membrane strains remain small. These are the crucial points that make the Kirchhoff-Love shell model [1] a viable choice which furthermore shall be computationally more efficient than the commonly used full 3D continuum models. The usual way to treat plasticity within a structural theory is the through-the-thickness integration approach [2] that superimposes the structural kinematics on a continuum element to perform a thickness integration of stress resultants by virtue of the elastic-plastic constitutive law treated in integration points. This method, which has been implemented for the roll forming process already [under review], is accurate but slow in comparison to the stress-resultant approach that aims for an implementation of elasto-plasticity on the structural level. In particular, the yield criterion and its evolution by means of a hardening law that properly resolves the continued plastification of the through-the-thickness element need to be formulated in terms of

the shell stress resultants and further state variables. In the present contribution we continue the development of a previously reported stress-resultant plasticity model [3] that is sufficiently accurate for elastic-plastic plate bending but requires improvements when proceeding to the geometrically nonlinear process of roll forming. The main advance of the here proposed stress-resultant plasticity model lies in the proper account for membrane forces and membrane plastic strains, which have a significant impact on the outcome of the forming process. All three approaches to handle the plastic behavior of a thin elastic-ideal-plastic metal sheet are implemented in a mixed Eulerian-Lagrangian shell finite element program to simulate the roll forming process. The comparisons of the new stress-resultant model against the previously reported one as well as against reference computations with the continuum plasticity model demonstrate the capabilities of the proposed scheme to accurately simulate the forming process at significantly reduced computational cost. [1] Eliseev, V.V., Vetyukov, Y.M. Finite deformation of thin shells in the context of analytical mechanics of material surfaces. [2] M. Ambati, J. Kiendl, L. De Lorenzis, Isogeometric Kirchhoff-Love shell formulation for elasto-plasticity. [3] E. Kocbay, Y. Vetyukov, Stress resultant plasticity for plate bending in the context of roll forming of sheet metal.

Nonlinear cable computations using high-order solid elements with hp-adaptive refinement for anisotropic plasticity

Hildebrandt-Raj, André *(Hamburg University of Technology, Germany)*
Sharma, Prateek *(Saarland University, Germany)*
Diebels, Stefan *(Saarland University, Germany)*
Düster, Alexander *(Hamburg University of Technology, Germany)*

09:30

In the modern world cables are an integral part of many engineering applications. They are used as tensile components in static structures such as bridges or buildings, but also in dynamic applications such as ski lifts and robots, or in the maritime industry. In addition to their structural use, cables are also used to transmit electrical power and signals in applications ranging from electric vehicles, aerospace industry to robotics. While structural cables typically have a twisted layout using steel or fabric as the material, this work focuses on the structural behaviour of electrical or signal processing cables with a parallel or coaxial internal structure. They pose a serious challenge as they are made up of several layers of material, including the copper wires, polymer and aluminium insulation, and a protective polymer jacket. Resolving their complex internal structure in a simulation is extremely costly as there is frictional contact between the components, which can lead to a geometric rearrangement of the parts. To overcome these challenges, the cable is represented by a single homogeneous effective material that exhibits anisotropies in both the elastic and elastoplastic domains [1]. The effective material properties for the anisotropic model are identified through experimental tension and torsion tests using the particle swarm optimisation method. Subsequently they are validated using free bending experiments with and without prior torsion applied and equivalent FEM simulations [2]. In order to perform accurate but efficient simulations, high-order solid elements with hierarchical shape functions [3] are used. They can be refined hierarchically and adaptively [4] to better resolve local phenomena such as contact interfaces,

boundary conditions, or evolving plasticity. Combined with quasi-regional mapping, curved geometries can be represented in great detail, while exhibiting large deformations with high local strains.

References

[1] Sansour, C., Karšaj, I., & Sorić, J., (2006). A formulation of anisotropic continuum elastoplasticity at finite strains. Part I: Modelling. *International journal of plasticity*, 22(12), 2346-2365.
[2] Hildebrandt, A., Sharma, P., Düster, A., & Diebels, S. (2022). Experimental and numerical investigation of the deformation behaviour of cables and thin beam-like structures under multi-axial loading. *Mathematics and Mechanics of Solids*, 27(10), 2314-2337.
[3] Hildebrandt, A., & Düster, A. (2022). Numerical Investigation of High-Order Solid Finite Elements for Anisotropic Finite Strain Problems. *International Journal of Computational Methods*, 19(05), 2250007.
[4] Zander, N., Bog, T., Kollmannsberger, S., Schillinger, D., & Rank, E. (2015). Multi-Level hp-Adaptivity: High-Order Mesh Adaptivity without the Difficulties of Constraining Hanging Nodes. *Computational Mechanics*, 55(3), 499-517.

A Proximal Newton Solver for Rate-Independent Formulations of Finite-Strain Plasticity

Jaap, Patrick *(TU Dresden, Germany)*
Pötzl, Bastian *(Universität Bayreuth, Germany)*
Sander, Oliver *(TU Dresden, Germany)*
Schiela, Anton *(Universität Bayreuth, Germany)*

09:50

Time discretization of the energetic rate-independent formulation of plasticity leads to a sequence of minimization problems in the space of deformations and plastic strains. In the finite-strain setting these problems are nonconvex. Furthermore, they are nonsmooth due to the rate-independent dissipation, and the common assumption of plastic incompressibility adds a further equality constraint. Nevertheless, the problems have important algebraic and geometric structure, which can be used to construct robust and efficient solvers. We approach the problem with a Proximal Newton method, which solves a sequence of intermediate problems that are coercive and convex, but still nonsmooth. Global convergence can be shown even if the intermediate problems are solved only inexactly. These intermediate problems have the same structure as small-strain primal plasticity problems. In particular, they are block-separable, and can be solved with a nonsmooth multigrid method such as TNNMG. Together, we obtain a globally convergent solver that reliably and efficiently handles situations with extreme strains.

Beams and frames with dissipative joints of shape memory material

Kuczma, Mieczyslaw *(Poznan University of Technology, Poland)*
Łasecka-Plura, Magdalena *(Poznan University of Technology, Poland)*
Tabrizikahou, Alireza *(Poznan University of Technology, Poland)*

10:10

The structural joints play a major role in the response of framed structures, members of which are commonly made of concrete, steel, timber, or combinations of these materials. The role of structural connections is especially evident in the circumstances of extreme loads caused by

a terrorist attack or natural disasters (explosive load, destruction of columns, earthquakes). In this contribution a computation model for beams and frames with joints made of pseudoelastic shape memory material will be presented. The model takes into account the hysteretic behaviour of the pseudoelastic shape memory material that is demonstrated in the form of the characteristic flag-type hysteresis loops in the stress-strain space, which are exhibited by shape memory alloys as a result of martensitic phase transformation. This class of active materials possesses the ability to undergo a large recoverable deformation upon the application of an external stimulus. The developed model is based on the simplifying assumption that the material nonlinear response is lumped in zones of energy dissipation, in a manner similar to the concept of the hinge in the theory of plasticity. Use is made of the Clausius-Duhem inequality in order to control the dissipation of energy during the deformation process, which allows us to consistently formulate the progress of martensitic phase transformation process in the joints as a complementarity problem. A computer program based on the finite element discretization is developed. Results of numerical simulations will be provided for the structural response of beams and frames with shape memory alloy joints, which illustrate also the self-centring property of this kind of structures.

S04-08: Structural mechanics

Date: June 2, 2023 11:00-13:00
Room: HSZ/AUDI

Nonlinear dynamic analysis of rods precluding shear and torsion with isogeometric discretizations

Nguyen, Thi-Hoa *(Technical University of Darmstadt, Germany)* 11:00
Roccia, Bruno A. *(University of Bergen, Norway)*
Hiemstra, René R. *(Technical University of Darmstadt, Germany)*
Gebhardt, Cristian G. *(University of Bergen, Norway)*
Schillinger, Dominik *(Technical University of Darmstadt, Germany)*

In this paper, we investigate, in the context of isogeometric analysis (IGA) [1], the recently developed formulation of nonlinear rods exhibiting only axial and bending deformations introduced in [2]. We utilize the higher-order continuity of smooth spline functions which naturally fulfill the C^1 continuity required by the nonlinear formulation of [2]. The number of discrete variable fields, compared to the standard spatial discretization scheme using cubic C^1 Hermite polynomials in the same reference, thus can be reduced. The resulting discrete solution belongs to $(R^3)^m$ that is larger than the manifold $(R^3 \times S^2)^n$ of the standard scheme, however, might not preserve the same manifold structure. Inspired by [2], we employ the implicit time integration scheme that is a hybrid combination of the midpoint and trapezoidal rules. It approximately preserves the energy and exactly preserves the linear angular momentum, and thus is efficient and robust for our investigation. We demonstrate, via two- and three-dimensional numerical examples of rods, that isogeometric discretizations of the same polynomial degree and smoothness are less robust than the standard spatial discretization scheme using Hermite polynomials. Their robustness can be improved by using, for instance, the strong approach of outlier removal, or by reducing the time step. We illustrate, via an example of a swinging rod under non- and conservative, and pulsating forces, that the improved discretization scheme thus can be employed for highly nonlinear cases. We also show that the configuration-dependent mass matrix of the studied formulation behaves irregularly and thus cannot be simplified to a configuration-independent one.

References:

[1] T. J. R. Hughes, J. A. Cottrell, Y. Bazilevs, Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement, Computer Methods in Applied Mechanics and Engineering 194 (39) (2005) 4135-4195.

[2] C. G. Gebhardt, I. Romero, On a nonlinear rod exhibiting only axial and bending deformations: mathematical modeling and numerical implementation, Acta Mechanica 232 (10) (2021) 3825-3847.

Simultaneous solution of ropes and membranes on all level sets within a bulk domain

Kaiser, Michael Wolfgang *(TU Graz, Austria)* 11:20
Fries, Thomas-Peter *(TU Graz, Austria)*

We formulate a mechanical model in the context of the finite strain theory for ropes and membranes which applies simultaneously to *all* level sets of a level set function over a prescribed bulk domain. The geometrically non-linear formulations are based on the tangential differential calculus [1]. Previous works only consider the *zero*-level set for the definition of *one* geometry [2]. Curvilinear coordinates which are usually used to describe curved structures, e.g., [3], do not apply in the present context. The co-area formula is used to formulate a weak form of the governing PDE. Similar approaches for other PDEs on manifolds, e.g., the Laplace-Beltrami operator, conservation and diffusion problems, can be found in [4] and references therein. To approximate the solution of implicitly defined ropes and membranes on the zero level set, the TraceFEM was used in [2]. Herein, we propose to discretize the bulk domain with higher-order elements and simultaneously solve for the displacements on all level-sets implied by some level-set function over the bulk domain. Such a method may be called Bulk-TraceFEM. To the best of our knowledge, it is the first time that this method, to approximate the solution of PDEs on manifolds, is used for curved geometries in structural mechanics. Higher-order convergence studies of numerical examples, based on the residual error, ensure the validity of this method and confirm optimal convergence rates. To further verify the proposed method, the stored elastic energy is compared with results obtained with the classical FEM based on a parametrization of the geometry of one single rope or membrane respectively.

[1] M. C. Delfour and J.-P. Zolésio, *Shapes and Geometries: Metrics, Analysis, Differential Calculus, and Optimization*. SIAM, Philadelphia, 2011.
[2] T.-P. Fries and D. Schöllhammer, A unified finite strain theory for membranes and ropes. *Comput. Methods Appl. Mech. Engrg.*, Vol. 365, p. 113031, 2020.
[3] Y. Başar and W. B. Krätzig, *Mechanik der Flächentragwerke*. Vieweg + Teubner, Braunschweig, 1985.
[4] G. Dziuk and C. M. Elliott, Finite element methods for surface PDEs, *Acta Numerica*, Vol. 22, p. 289-396, 2013.

Towards realistic nonlinear elastic bending behavior for cable simulation

Zhao, Tian *(Fraunhofer Institute for Industrial Mathematics ITWM; Technical University of Darmstadt)* 11:40
Schneider-Jung, Fabio *(Fraunhofer Institute for Industrial Mathematics ITWM)*
Linn, Joachim *(Fraunhofer Institute for Industrial Mathematics ITWM)*
Müller, Ralf *(Technical University of Darmstadt)*

To simulate slender flexible structures such as cables and hoses, Cosserat rod theory provides a suitable framework for efficient and geometrically exact modeling [1]. For many applications, a linear elastic constitutive model, i.e. a constant bending stiffness, is sufficient to simulate the bending behavior. However, for more complex structures, the nonlinear elastic behavior is necessary to be considered. In our recent work [2], we introduced an iterative method to enable the nonlinear elastic behavior of cables in our framework of using Cosserat

rod theory [1], where static equilibrium states of rods under given boundary conditions are obtained by minimizing the potential energy. In this method, we update the local bending stiffness constants according to a given characteristic iteratively, until the energy minimum is reached. Moreover, we formulated a corresponding inverse problem to determine the nonlinear elastic properties, i.e. a state-dependent bending stiffness characteristic for given measurement data. In this contribution, we further present the enhancement of the inverse problem by including the pre-curvature as an additional optimization variable. Additionally, we propose an alternative method to identify the bending stiffness characteristic based on the balance equations for rods in static equilibrium. We perform numerical examples to validate both methods and then apply them to experimentally measured data. Finally, the results obtained from both methods are compared and discussed.

[1] J. Linn, T. Hermansson, F. Andersson, and F. Schneider. Kinetic aspects of discrete Cosserat rods based on the difference geometry of framed curves. In: M. Valasek, et al. (eds) Proceedings of the ECCOMAS Thematic Conference on Multibody Dynamics, 163-176. Prague, Czech Republic, 2017.
[2] T. Zhao, F. Schneider-Jung, J. Linn and R. Müller. Simulating nonlinear elastic behaviour of cables using an iterative method. In ECCOMAS Congress 2022-8th European Congress on Computational Methods in Applied Sciences and Engineering, 2022.

Experimental investigation of cables and its components under multi-directional loading

Sharma, Prateek *(Saarland University, Germany)*
Hildebrandt-Raj, André *(Hamburg University of Technology, Germany)*
Düster, Alexander *(Hamburg University of Technology, Germany)*
Diebels, Stefan *(Saarland University, Germany)*

12:00

With increase in electro-mobility the use cables in automobiles has increased manifolds. Along with that, the use of robots in industry has also resulted in the increased use of cables. They are then not only used as electrical conductor but also as structural elements. Their lifetime depends on how much mechanical loads are applied on them. Therefore, apart from their electrical capabilities it is important to characterise them mechanically.
Different constituents such as wires and insulation make up a cable. These components can interact with each other and either hinder the movement of the other components or dissipate energy due to the friction between them. The type and direction of loading, therefore, influences the mechanical response of the cable. In tensile direction, for example, a cable is much stiffer than in the bending and torsion direction.
In this work, the cable is tested in tensile, torsion and bending direction for a complete mechanical characterisation. To test the effect of the interaction between its components, a cable is deconstructed layer by layer and then characterised. With this the effect of the interaction between the insulation and the inner core is studied. For a coaxial cable, an increase in the tensile stiffness can be noted as the outer layers are removed. This suggests a slip between the insulation and inner core. To understand the interaction between the wires within a cable, torsion tests were conducted in both clockwise and anti-clockwise direction. A drastic difference between the stiffness in both the directions can be seen in the first cycle of loading.

However, with further loading the difference reduces, suggesting a reorientation of wires as the loading continues. Thus, an experimental characterisation of cables and its components under different loading conditions is presented.

Experimental investigations of the dynamic behaviour of high-voltage cables in electric trucks

Volltrauer, Jan *(Daimler Truck AG, NVH Entire Vehicle, Germany)*
Buck, Fabian *(Daimler Truck AG, NVH Entire Vehicle, Germany)*
Fründ, Eckhard *(Daimler Truck AG, NVH Entire Vehicle, Germany)*
Hetzler, Hartmut *(University of Kassel, Institute of Mechanics, Engineering Dynamics Group)*
Bäuerle, Simon *(University of Kassel, Institute of Mechanics, Engineering Dynamics Group)*

12:20

Electromobility is one of this decade's most important topics. In order to reduce emissions, the EU sets targets for limits on the amount of CO2 emitted by heavy-duty vehicles [1]. For this reason, trucks with alternative drive systems, especially electric trucks, are being developed to an increasing extent. Simulations take a crucial role in current product development processes. For an accurate representation of the dynamic behaviour of electic trucks, the influence of the high-voltage cables is investigated to provide a basis for minimal substitute models. Different modelling approaches for cables can be found in literature: Lv et al. [2] provide an overview of techniques used for cable modelling. A fundamental investigation of the properties of high-voltage cables is given by Bönig [3]. For the investigation of the dynamic properties of the cables, a test bench is set up to enable a realistic installation of high-voltage cables. Different cable variations (length, number, shape), clamping situations and excitation types are examined in order to classify the overall cable behaviour. The evaluation is carried out by determined frequency response functions. The parameter values of mass, stiffness and damping of a linear single-degree-of-freedom oscillator, which is used as the mechanical substitute model, are extracted. The cable has a major influence on the dynamic behaviour of the test bench: By integrating cables, a significantly greater damping is achieved than without cables. Likewise, the natural frequency of the system changes due to the added stiffness. Both reducing the cable length and adding more cables increases the system's stiffness and damping. The shape of the cable strongly changes the parameter values, whereas the selected clamping conditions have only a minor influence. The behaviour of the cable cannot be fully represented by the linear model with regard to different excitation strengths: The cable exhibits degressive stiffness and damping behaviour; however, at higher frequencies the damping is progressive. The nonlinear behaviour can be represented by extending the linear model to include higher order polynomial stiffness and damping parameters. Reasons for the nonlinearity may be due to the clamping or the design of the cable.

[1] Europäisches Parlament und Europäischer Rat. "VERORDNUNG (EU) 2019/1242" (2019). https://eur-lex.europa.eu/legal-content/de/TXT/?uri=CELEX%3A32019R1242.
[2] N. Lv, J. Liu, H. Xia, J. Ma und X. Yang, "A review of techniques for modeling flexible cables", Computer-Aided Design (2020).
[3] J. Bönig, "Integration des Systemverhaltens von Automobil-Hochvoltleitungen in die virtuelle

Absicherung durch strukturmechanische Simulation", Friedrich-Alexander-Universität Erlangen-Nürnberg (2016).

Economic fatigue damage monitoring for vehicle fleets using the scattering transform

Heindel, Leonhard *(Technische Universität Dresden, Germany)* 12:40
Hantschke, Peter *(Technische Universität Dresden, Germany; Dresden Center for Fatigue and Reliability (DCFR))*
Kästner, Markus *(Technische Universität Dresden, Germany; Dresden Center for Fatigue and Reliability (DCFR))*

Vehicles are designed to endure a specific load collective, which encompasses the different usage scenarios that are expected to occur during the lifetime of the vehicle. Due to the individual preferences and needs of customers, real usage can strongly deviate from this load collective. Information on the history of fatigue development for any given vehicle would enable predictive maintenance approaches, where critical components can be replaced before their expected point of failure. In order to implement fatigue monitoring in an economic manner, a virtual sensing approach is used where an exhaustive sensor setup is only required for few vehicles in a fleet.
The scattering transform [1] has been successfully applied to audio and image classification as well as earthquake detection [2]. Here, it is used to extract coefficients from measurement data, which are invariant to translation and stable to time shifting deformation. These features are further compressed using principal component analysis, leading to a low dimensional representation of the sensor measurements. This representation contains compact information on the history of the vehicle's dynamic state, which can be used for fatigue monitoring.
The approach is demonstrated using measurement data from a sensor equipped eBike [3]. Few acceleration sensors are used to infer the general dynamic state of the vehicle, while a large number of strain gauges provide local, fatigue critical information. The scattering transform is employed to obtain the reduced data representation of the acceleration sensors. A strong correlation between exists the resulting principal components and the fatigue damage data from strain gauges measurements, enabling a direct regression approach. In addition, a small number of additional measurements for specific eBike maneuvers allow for a physical interpretation of the principal component representation.

References:

[1] J. Andén and S. Mallat, Deep Scattering Spectrum. IEEE Transactions on Signal Processing, vol. 62, no. 16, pp. 4114-4128, 2014
[2] L. Seydoux, R. Balestriero, P. Poli, et al. Clustering earthquake signals and background noises in continuous seismic data with unsupervised deep learning. Nat Commun 11, 3972, 2020
[3] L. Heindel, P. Hantschke and M. Kästner Fatigue monitoring and maneuver identification for vehicle fleets using a virtual sensing approach, International Journal of Fatigue, Volume 170, 2023

S04-09: Structural mechanics

Date: June 2, 2023 11:00-13:00
Room: HSZ/201

Out-of-plane buckling and dynamic instability of an axially moving flat Euler-Bernoulli beam under the action of in-plane distributed forces

Scheidl, Jakob *(TU Wien, Austria)* 11:00
Steindl, Alois *(TU Wien, Austria)*

We consider the problem of a moving flat blade loaded by in-plane distributed forces that induce bending of the travelling structure in the plane of maximum flexural rigidity and, thus, render it susceptible to torsional flexural buckling. Previous works on this topic with relation to the operation of band saw blades were concerned with static divergence buckling and dynamic vibrations of wide blades modelled with plate theory. We employ the general three-dimensional theory of an unshearable Euler-Bernoulli beam including torsion to address the dynamic stability problem. Warping need not be considered due to the rectangular cross-section being quasi-warping free, but the stiffening of the torsional rigidity due to axial pre-tensioning – sometimes referred to as Wagner effect – is consistently accounted for. Furthermore, the eccentric action of the distributed transverse forces on the side edges of the blade give rise to distributed moments with respect to the beam axis. Contrary to preceding studies, we emanate from the full nonlinear governing equations to deduce the linearised system of governing equations about the stationary motion by means of an expansion in a small parameter. This formal approach shall aid the extension of the present study to a full nonlinear stability analysis in the future. To this end, we perform a classic stability analysis in the framework of the second order theory of the pre-stressed axially-moving blade. Critical points relate to torsional flexural buckling and dynamic instability of the axially moving blade.

An energy-based finite-strain constitutive model for bent heterostructured materials

Hadjimichael, Yiannis *(Weierstrass Institute, Germany)* 11:20
Merdon, Christian *(Weierstrass Institute, Germany)*
Farrell, Patricio *(Weierstrass Institute, Germany)*
Liero, Matthias *(Weierstrass Institute, Germany)*

In this talk, we present a comprehensive study of the mechanical behavior of bent heterostructures. Bent heterostructures are important materials due to their augmented electronic and optical properties resulting from combining two or more materials. This combination introduces strain and modifies the electronic band structure and the behavior of charge carriers, making them attractive for various applications in fields such as photonics, electronics, energy, and biotechnology.

To better understand the mechanical behavior of bent heterostructures, we propose a constitutive model for nonlinearly elastic heterostructured materials that considers the presence of a local intrinsic prestrain. The prestrain is a function of the mismatch of lattice constants between the composite materials. This model is based on an energy functional that depends

on a multiplicative decomposition of the deformation gradient, the prestrain, and varies in each composite domain. The resulting PDE system in Lagrangian coordinates is nonlinear, although we use a linear relation between stress and strain via Hooke's law.

To validate our model, we apply it to bimetallic beams and hexagonal heteronanowires and perform numerical simulations using finite element methods (FEM). Our simulations examine how the structures bend for different material compositions and cross-section geometries. We also compare the bending curvature with analytic derivations to assess the model's validity and the accuracy of the simulations. The analytic expressions are formulated using a kinetic framework and taking into account the lattice constant difference across the material interface of the composite. Our findings provide valuable insights into strained bent heterostructures and contribute to the study of structures with enhanced electronic and optical properties.

Dynamic response of frames with viscoelastic dampers under uncertain parameters

Łasecka-Plura, Magdalena *(Poznan University of Technology, Poland)* 11:40

In structural analysis, it is most often assumed that the design parameters have precisely defined values. However, the real ones may differ from the assumed, and failure to take this fact into account in the design process may lead to large differences between the calculated response of the structure and the real one.

Methods that take into account the uncertainties of design parameters can be divided into those assuming a random distribution of parameters or changing parameters only within certain limits. In the second case, interval analysis [1] can be used for calculations. This paper presents a method for calculating the frequency response function (FRF), which is often used in the analysis of the dynamic response of the structure. Various approaches to this problem can be found in [2-4].

In this paper, in the first step, the equations of motion of structures with uncertain design parameters are written. Then, after applying the Fourier transformation, a linear system of interval equations to be solved is obtained. The solution to this system is the FRF, which is obtained using Brower's fixed point theorem [3].

A shear frame with built-in viscoelastic dampers is considered. The behavior of dampers is described using both classical and fractional rheological models. Design parameters are assumed to vary independently. In this paper, in order to eliminate the unfavorable overestimation of the results resulting from the calculus of interval numbers, the equations of motion are written using the element-by-element method. This eliminates the overlapping of the influences of two or more uncertain parameters. The obtained results are compared with the vertex method, and the results obtained using direct calculus of interval numbers. Various parameter variations are considered to determine the effectiveness of the proposed method.

[1] Moore, R. E., Methods and applications of interval analysis. London: Prentice-Hall, Inc, 1979.

[2] Muscolino G., Santoro R., Sofi A., Explicit frequency response functions of discretized structures with uncertain parameters. Computers and Structures, 2014, 133:64-78.

[3] Yaowen, Y., Zhenhan, C., Yu, L., Interval analysis of frequency response functions of structures with uncertain parameters. Mechanics Research Communications, 2013, 47:24-31.

[4] Łasecka-Plura M., Lewandowski R., Dynamic characteristics and frequency response function for frame with dampers with uncertain design parameters, Mechanics based design of structures and machines, 2017, 45 (3):296-312.

A practicable approach for stability analysis in soft robotics

Seis, Robin *(RPTU Kaiserslautern - Landau, Germany)* 12:00
Lamping, Frederik *(RPTU Kaiserslautern - Landau, Germany)*
de Payrebrune, Kristin M. *(RPTU Kaiserslautern - Landau, Germany)*

Soft robotics is a novel field in robotics that has gained importance in recent years. The idea in soft robotics is to use materials with a softness comparable to human tissue. With these materials, soft robots are capable to adapt to their environment without extensive use a of sensor system. This makes them interesting, for example, in rehabilitation or as a surgery tool. Due to their softness, soft robots are typically underactuated, which means that they have a lower number of actuators than degrees of freedom. For practical applications, it is important to determine the workspace of a robot and its stability limits, and to identify the design parameters that affect it. Due to the underactuation, this is more challenging than for "classical" robots. Two common approaches can be found in literature. Either an analytical model of the robot is examined for singularities, or a phenomenological investigation is done by performing simulations. We propose to use a combination of both approaches and, thus, to benefit of the advantages of both. In particular, the advantage of using an analytical model simplifies to analyze the influence of individual design parameters on the workspace and stability limits. However, finding a suitable analytical model of the robot can be challenging. In contrast, the simulative approach is less challenging to perform, but is less general, since it suffers the possibility to analyze the influence of individual design parameters. With our combined approach, analysis of the influence of individual design parameters becomes possible, but the requirements for the model are lower than for a pure analytical approach. We are able to determine the workspace and stability limits of various robots with only limited effort. Consequently, building robots customized to perform a certain task becomes possible.

Experimental and simulation-based modeling of a vehicle seat

Wagner, Philipp *(BMW Group, Germany)* 12:20

The automotive industry must deal with great challenges in future. Consequently, the prediction of the Noise-Vibration-Harshness (NVH) in early design and concept phase becomes an important role. Especially dynamic seat behavior has an immediate effect to the ride comfort and hence of the customer acceptance. Therefore, it is important to have reliable finite element (FE) models for the simulation-based prediction of the dynamic seat behavior. In this study different aspect of the experimental and simulation-based modeling of a vehicle seat are described. The experimental modal analysis is used to characterize the seat system as well as the subsystems seat backrest and seat frame. Consequently, the structure dynamic behavior of a seat depends on manifold sensitive parameter. The FE-models are validated

based on these measurements. Furthermore, are the measurement used to identifying the main vibration contributor to the full seat system. Thus, findings are utilized to improve the predictive power of simulation results.

Lévy-type solutions for buckling of shear deformable unsymmetrically laminated plates with rotational restraints

Schreiber, Philip *(Technische Universität Darmstadt, Germany)* 12:40
Mittelstedt, Christian *(Technische Universität Darmstadt, Germany)*

The local stability of unsymmetric laminated structures is significantly affected by bending-extension coupling and the comparatively low transverse shear stiffnesses, which have to be included in the structural analysis. If such structures have flat surfaces in segments, they can be investigated with the discrete plate analysis. In this analysis, the individual segments are considered as plates with rotational restraints which represent the supporting effect of the surrounding structure.

The aim of this work is to improve the analytical stability of laminated plates. Therefore, Lévy-type solutions for the buckling load of the mentioned laminated plates are considered and refined. This offers exact solutions for unsymmetrical cross-ply laminates as well as anti-symmetric angle-ply laminates. In order to show the influence of shear deformations, the solutions for Classical Laminated Plate Theory (CLPT), First-order Shear Deformation Theory (FSDT), and Third-order Shear Deformation Theory (TSDT) are worked out and compared to each other. In the context of TSDT, a new formulation for the rotational elastic restraint is presented, which affects the rotation and the warping of the plate cross-section.

This investigation presents the influence of shear deformations on different laminates and classifies the benefits of the different laminated plate theories with respect to the stability behaviour under different boundary conditions. In addition, the influence of bending-extension coupling on different fibre angles and layer sequences is analysed.

S04-10: Structural mechanics

Date: June 2, 2023 16:00-18:00
Room: HSZ/AUDI

Multi-level Bézier extraction of truncated hierarchical B-splines for isogeometric analysis

Grendas, Andreas *(TU Graz, Austria)* 16:00
Marussig, Benjamin *(TU Graz, Austria)*

Isogeometric analysis (IGA) models lack adaptivity due to the tensor product structure of B-splines and Non-uniform rational B-splines (NURBS). Truncated hierarchical B-splines (THB-splines) provide a solution for this. THB-splines organize the parameter space into a hierarchical structure, which enables efficient approximation and representation of functions with different levels of detail. The truncation mechanism ensures the partition of unity property of B-splines and defines a more scattered set of basis functions without overlapping on the multi-level spline space. Following, with the Bézier extraction method to specify the globally defined spline functions into Bézier elements, provide an element structure for isogeometric analysis that can be easily incorporated into existing finite element codes, without any changes. The Bézier extraction operator enables numerical integration of smooth functions to be performed on C^0 Bézier elements. By separating the multi-level extraction of the THB-splines from the standard Bezier extraction, a more general independent framework applicable to any sequence of nested spaces is created. Both approaches preserve the element-local concept used in standard finite-element implementations for the analysis algorithms. The operators for the multi-level structure of THB-splines and the operators of Bézier extraction are separated for each element of the basis. This presented implementation involves the use of an open-source Octave/MATLAB code called GeoPDEs [1]. By adjusting the operators for the multi-level structure from an element point of view and multiplying with the Bézier extraction operators in an element-wise approach as well, we create Bézier elements in a multi-level spline space and solve using the element-based solvers of GeoPDEs. Several examples are presented to investigate the performance of multi-level Bézier extraction with a standard THB-spline approach.

[1] E. M. Garau and R. Vázquez, Algorithms for the implementation of adaptive isogeometric methods using hierarchical B-splines, *Applied Numerical Mathematics,* p. 58-87, 2018.

Transient Response of Pavement Structures Under Moving Wheel Loads Using the ALE Methodology

Anantheswar, Atul *(Technische Universität Dresden, Germany)* 16:20
Wollny, Ines *(Technische Universität Dresden, Germany)*
Kaliske, Michael *(Technische Universität Dresden, Germany)*

The dynamic response of long structures (e.g., pavements) subjected to moving loads, is generally difficult to simulate using conventional methods like the finite element method in the Lagrangian setting. This is because the entire length of the structure that is in the path of the moving load would need to be discretized, and this in turn would require large meshes. Additionally, if improvement in quality of results through the use of finer mesh sizes is sought, the entire region of the mesh in the load path would require refinement. As a direct result,

long simulation run-times can be expected when using conventional methods. To overcome these drawbacks, and improve the efficiency of the finite element simulations, the Arbitrary Lagrangian Eulerian (ALE) approach can be used to simulate pavement structures, provided longitudinal homogeneity is assumed [1]. Typically, ALE formulations are used in adaptive meshing strategies [2]. However, the ALE formulation has been adapted to be capable of simulating the quasi-static response of pavement structures [1]. This contribution uses an extension of the quasi-static ALE framework to the transient domain, enabling the study of the dynamic response of pavement structures subjected to moving loads. The central idea behind this framework is a change in perspective. In this new perspective, the observer moves with the load. Hence, the load appears to always have a constant location, while the material appears to flow under the load. With this concept, it becomes feasible to obtain the same response of the material to the applied load, as with conventional methods, while only simulating a significantly smaller region around the load. This greatly reduces computational effort, because fewer finite elements are required. Additionally, it becomes easier to apply finer meshes around the load, as it appears to be fixed in position from the ALE perspective. In this work, some case studies are considered to highlight the capabilities of this dynamic ALE framework.

References

[1] Wollny, I., & Kaliske, M. (2013). Numerical simulation of pavement structures with inelastic material behaviour under rolling tyres based on an arbitrary Lagrangian Eulerian (ALE) formulation. *Road Materials and Pavement Design*, *14*(1), 71-89.

[2] Zreid, I., Behnke, R., & Kaliske, M. (2021). ALE formulation for thermomechanical inelastic material models applied to tire forming and curing simulations. *Computational Mechanics*, *67*(6), 1543-1557.

Monolithic FE² approach for thermomechanical modeling of beam structures

Klarmann, Simon *(Chair of Structural Analysis and Dynamics, RWTH Aachen University, 52062 Aachen, Germany)*
Gebhart, Philipp *(Institute of Solid Mechanics, Technische Universität Dresden, 01062 Dresden, Germany)*
Wallmersperger, Thomas *(Institute of Solid Mechanics, Technische Universität Dresden, 01062 Dresden, Germany)*
Klinkel, Sven *(Chair of Structural Analysis and Dynamics, RWTH Aachen University, 52062 Aachen, Germany)*

16:40

In the present contribution, the FE^2 scheme for beam elements is extended to thermomechanically coupled problems. Beam elements have the advantage of drastically reducing the number of degrees of freedom compared to solid elements. However, the major challenge in modeling structures with beam elements lies in developing sophisticated non-linear beam material models. This drawback resides in the fact that these elements require effective cross-sectional properties involving material and geometric properties. The FE^2 method, combined with a homogenization scheme based on the Hill-Mandel condition, solves this problem. Within this scheme, homogenization of a representative volume element (RVE) on the mesoscopic scale provides effective cross-sectional properties for the macroscopic scale.

This homogenization procedure allows the consideration of non-linear material formulations and cross-sectional deformation within the analysis of a beam structure. The applicability of such a FE^2 scheme for purely mechanical problems was already shown. In the present contribution, an extension to thermomechanically coupled problems is provided. In the proposed setting, the macroscopic scale is represented by beam elements with displacement, rotation, and temperature degrees of freedom. Solid elements with displacements and temperature degrees of freedom describe the behavior of the RVE. Hence, the proposed extension solves both scales in a monolithic approach. The assumption of a steady state problem at both scales allows a focus on a consistent scale transition and a discussion about the choice of suitable boundary conditions under the assumption of beam kinematics.

Method of Manufactured Solutions in the Context of Embedded Domain Simulations

Petö, Márton *(Otto von Guericke University Magdeburg, Germany)* 17:00
Duvigneau, Fabian *(Otto von Guericke University Magdeburg, Germany)*
Eisenträger, Sascha *(Darmstadt Technical University)*
Juhre, Daniel *(Otto von Guericke University Magdeburg, Germany)*

Code verification plays a crucial role in finite element applications, especially in embedded domain methods, where the typically complex geometric domain is immersed into an easily discretizable larger domain, and the original problem is solved using an unfitted mesh [1]. These methods deal with some unique numerical and algorithmic challenges and are often based on novel algorithms and error-prone in-house codes. Thus, reliable and easy testing of the different features used in these methods is of significant importance. Oftentimes, this is carried out by testing the numerical solutions against some reference solutions, which are either obtained by overkill finite element approximations or by readily available analytical solutions. While the first approach requires additional time investment and FEM resources, the second approach is only available in the simplest cases.

The method of manufactured solutions (MoMS) constitutes a third approach, which, by utilizing a simple trick, enables an easy and straightforward derivation of closed-form reference solutions: Instead of trying to solve a given partial differential equation analytically, one manufactures a solution, whose spatial and time derivatives are known. This can be easily inserted into the strong form of the mathematical problem to compute the source term analytically. In case of a correct implementation of the numerical approach, the source term acting in the problem domain, and appropriate boundary conditions on its boundary, should lead to an approximate solution that converges to the manufactured reference solution [2].

In our contribution, the application of the MoMS to embedded domain problems is of focus, where due to the complex geometric features and unfitted discretization, additional care is required when deriving manufactured solutions. As an established representative for immersed boundary approaches, we use the finite cell method, and with a series of 2D and 3D numerical examples, we demonstrate the code-testing capabilities of the MoMS for static and transient problems, involving void regions and single/multiple inclusions.

[1] J. Parvizian, A. Düster, and E. Rank. Finite cell method *h*- and *p*-extension for embedded domain problems in solid mechanics. Computational Mechanics, 41:121-133, 2007.

[2] K. Salari and P. Knupp. Code verification by the method of manufactured solutions. Technical Report, 2000.

Use of differential forms in the determination of differentials of cross products of tensors in nonlinear solid mechanics

Flajs, Rado *(University of Ljubljana, Faculty of Civil and Geodetic Engineering, Slovenia)* 17:20

We consider the cross product of tensors introduced by R. de Boer (1982) and used by J. Bonet et al. in the description of large strains solid mechanics (2016). From the contribution of J. Bonet et al. it appears that the cross product of tensors can be used to rearrange the mechanical descriptions and to simplify considerably the expressions of selected mechanical quantities encountered in the description of mechanical problems in large strains solid mechanics.

In this work, we derive some additional properties of the cross product of tensors that also allow some simplifications of selected mechanical quantities. In particular, we establish a connection between the cross product of operators and differential forms introduced by M. Spivak (1975, 2018). These connections allow further generalization of some expressions.

At this point we take advantage of the important fact that the second differentials of differential forms are zeros. This fact allows further simplification of certain expressions and opens further new possibilities in the description of mechanical problems in nonlinear solid mechanics.

References:

1. R. de Boer. Vektor-und Tensorrechnung für Ingenieure. (1982): 318-339.
2. J. Bonet, A. J. Gil, and R. Ortigosa. On a tensor cross product based formulation of large strain solid mechanics. *International Journal of Solids and Structures* 84 (2016): 49-63.
3. M. Spivak. *Differential Geometry, vol. 1*, Berkeley, California, USA: Publish or Perish. (1975).
4. M. Spivak. *Calculus on manifolds: a modern approach to classical theorems of advanced calculus*. CRC press, (2018).

Simulation of the mechanical behavior of coated particles using DEM-BPM

Safdar, Wasif *(Hamburg University of Technology, Germany)* 17:40
Rotter, Sonja *(Hamburg University of Technology, Germany)*
Heinrich, Stefan *(Hamburg University of Technology, Germany)*
Düster, Alexander *(Hamburg University of Technology, Germany)*

The collision of ships is still a significant cause of accidents, which have disastrous environmental consequences, such as oil spillage from oil tankers. Improving the crashworthiness of ship structural design is therefore important. One approach is to fill the double hull structure with granular material, as particle breakage helps to absorb kinetic energy and transfer the load from the outer to the inner hull [1]. To optimize the kinetic energy absorption and assess their suitability as crash absorbers, the particles can be coated with environmentally friendly materials [2]. However, the mechanical behavior is dependent on the type of coating material, making it challenging to set up a numerical model for simulation. An open-source Discrete Element Method code, MUSEN, is used to model coated particles numerically, which can be extended using the Bonded Particle Method to simulate particle breakage through solid bridges [3].

As the model consists of coating material as well as the primary particles, the number of parameters increases, as does the computational time. A robust methodology is needed to characterize the mechanical behavior regardless of the coating material type. Sensitivity analyses and parametric studies are conducted to study the effect of input parameters and determine the influential ones. This is followed by optimization of the remaining parameters using algorithms, such as the Particle Swarm Algorithm, validated against results from single particle compression tests. The optimized model is also compared with results from multi particle compression tests to determine its suitability in describing the mechanical behavior at the multi particle scale. The results from these simulations will be presented in this contribution.

[1] Schöttelndreyer, M. (2015): Füllstoffe in der Konstruktion: Ein Konzept zur Verstärkung von Schiffsseitenhüllen. Dissertation, Institut für Konstruktion und Festigkeit von Schiffen, Technische Universität Hamburg-Harburg.
[2] Orth, M., Rotter, S., Safdar, W., Tasdemir, S., Pietsch-Braune, S., Heinrich, S., & Düster, A. (2023). Fluidized Bed Spray Coating for Improved Mechanical Properties of Particles. *Processes*, *11*(2), 314. MDPI AG.
[3] Dosta, M. and Skorych, V. (2020): MUSEN: An open-source framework for GPU- accelerated DEM simulations. SoftwareX, Volume 12, 100618.

S05: Nonlinear oscillations

Organizer(s): **Hetzler, Hartmut** *(U Kassel)*
Dohnal, Fadi *(UMIT Tirol)*

S05-01: Nonlinear oscillations

Date: May 30, 2023 13:30-16:10
Room: CHE/183

Internal resonance in nonlinear structures and what it can be used for

Tatzko, Sebastian *(Leibniz Universität Hannover, Germany)* 13:30

In vibrating structures, nonlinear effects can play a decisive role. For example, stiffening responses can occur in integral components with low damping, but also softening effects with a shift of the resonance to lower values by an increase of the vibration energy can be observed. Often these systems are considered only in a characteristic nonlinear vibration mode, allowing well-known phenomena to be investigated. However, it may be the case that more than one nonlinear mode has a significant effect on the structural response of multi-degree-of-freedom systems. If these modes take on integer multiples of frequency values, we speak of an internal resonance.
In this presentation, the phenomenon of internal resonance is explained on the basis of a two-mass oscillator. For this purpose, nonlinear modal analysis is used to determine the amplitude-dependent behavior of the resonant frequencies, referred to as nonlinear modes. These nonlinear modes already display the internal resonance in the form of characteristic trajectories, which are examined and explained in more detail here. A computational framework consisting of Harmonic Balance and continuation is used to calculate the nonlinear mode curves. In addition, nonlinear frequency responses are determined and their trajectories and properties in the internal resonance region are shown. To further understand the oscillatory behavior animations are considered. Finally, a possible use for the observed properties is discussed as well as current approaches in research for the use of internal resonances are pointed out.

Nonlinear Dynamics and Machine Learning

Stender, Merten *(Technische Universität Berlin, Germany)*
Ohlsen, Jakob *(Hamburg University of Technology, Germany)*
Wedler, Mathies *(Hamburg University of Technology, Germany)*
Ehlers, Svenja *(Hamburg University of Technology, Germany)*
Punsmann, Emma *(Ruhr Universität Bochum)*
Luig, Björn *(University of Münster)* 14:10

The omnipresence of data-driven and learning-based approaches is evident across many research fields, and lately also in the field of nonlinear dynamics. This talk addresses application scenarios, challenges, and limitations for a range of machine learning-related approaches to nonlinear dynamics. Focus is put on i) deep black-box recurrent networks for behavior prediction, ii) fully convolutional multi-scale networks for data fusion and time stepping, and

iii) physics-informed approaches that leverage a-priori knowledge of the underlying process structure. While the latter approaches employ neural architectures for system identification and future state prediction, reservoir computing is presented to illustrate how a nonlinear dynamical system can be used for machine learning purposes. An outlook into physical reservoir computing is given, which makes use of physical devices for low-energy computing, but still requires a large amount of transdisciplinary research efforts.

On Functional Observers for Polynomial Systems with Nonlinear Oscillations

Röbenack, Klaus *(TU Dresden, Germany)*
Gerbet, Daniel *(TU Dresden, Germany)*
14:50

A state observer recovers the system's state from measured output. In some applications, not the full state information is needed but only a function of the state. In these cases one can use a functional observer. For linear time-invariant systems, existence conditions for both full state and functional observers are well-known. For nonlinear systems, there are different observability concepts. Even if a nonlinear system is locally or globally observable, the design of an observer is not straightforward. In this contribution we discuss the design of functional observers for polynomial systems. Our approach is based on a high gain design employing an embedded observer. The functional to be estimated is generated from the high gain observer's state. The restriction to polynomial systems allows the representation of the system's and the observer's dynamics as polynomial ideals. For our calculations we utilize methods from algebraic geometry. The method is illustrated on some chaotic systems.

Sparse identification of the dynamics of a nonlinear multistable oscillator

Kamecke, Steffen *(TU Berlin, Germany)*
Wulff, Paul *(TU Berlin, Germany)*
Gräbner, Nils *(TU Berlin, Germany)*
von Wagner, Utz *(TU Berlin, Germany)*
15:10

Recently data-driven modeling approaches are getting increasingly examined regarding their applicability for nonlinear mechanical or mechatronic systems. With a high data availability and often insufficiently accurate descriptions of complex behavior of real systems using established physical models, statistical models provide promising alternatives.

Alongside machine learning techniques like deep neural networks, regression is considered to obtain models from measurement data [1, 2]. With sparse regression, governing equations are estimated from a given function space so that the data is explained with as few terms as possible while maintaining a low model error. This method is implemented in a framework called Sparse Identification of Nonlinear Dynamics (SINDy) [1].

The current presentation succeeding from the Master thesis of the first author [3] and prior work of the chair on the application of sparse identification on a bistable energy harvesting system [2] demonstrates the application of these methods on free and forced vibrations of a one or two degree of freedom nonlinear rotary oscillators with multiple stable equilibrium positions. The setup and data acquisition as well as the application of sparse identification is described.

The selected function space containing the candidates is essential for an accurate representation of the system at hand. Monomials form a commonly used function space since they can approximate a wide variety of nonlinear characteristics. However, in this work, it is shown that monomials alone can be insufficient when friction is prominent. Therefore, to account for Coulomb friction corresponding functions are added as candidates to the function space of monomials up to the 5^{th} order. Adaptions of the common optimization algorithms turned out to be necessary for the inclusion of Coulomb friction.

As a result, it is found that the addition of a candidate for Coulomb friction increases the model quality significantly.

[1] Brunton, S. L.; Proctor, J. L.; Kutz, J. N.; Bialek, W.: Discovering governing equations from data by sparse identification of nonlinear dynamical systems. Proceedings of the National Academy of Sciences of the United States of America 113(15), 3932 - 3937, 2016.
[2] Wulff, P.; Lentz, L.; von Wagner, U.: Determination of the polynomial restoring force of a one DoF bistable Duffing oscillator by linear regression. Acta Mechanica 157, 2023.
[3] Kamecke, S.: Datenbasierte Modellierung eines harmonisch angeregten, nichtlinearen Drehschwingers mit zwei Freiheitsgraden, TU Berlin, master's thesis, 2022

Stability analyses for Hill Equation by the Homotopy perturbation method

Ramirez Barrios, Miguel Luis *(Unidad Profesional Interdisciplinaria de Biotecnología, Instituto Politécnico Nacional; Research Center for Microtechnology, Vorarlberg University of Applied Sciences)*
Dohnal, Fadi *(Research Center for Microtechnology, Vorarlberg University of Applied Sciences)*

15:30

Hill's equation is a second-order differential equation with real and periodic parameters, namely x"(t) + cx'(t) + (a+bv(t))x = 0 with v(t+T) = v(t). A vast of publication deals with its stability analysis. Two powerful theories describe Hill's equations dynamics: the so-called Floquet theory and the perturbations methods (Poincaré-Lindstetd, averaging, multiple scales, among others). The first is restricted to using numerical methods to integrate the equation, and the second is mandatory to assume a small parameter. On the other hand, the homotopy perturbation method has recently been used to describe a range of nonlinear and linear oscillation problems, presenting a considerable advantage: the homotopy analysis method is independent of any small or large quantities.

The stability of solutions of Hill's equation usually is represented as the so-called Ince-Strutt diagram, which consists of stable and unstable regions divided by transition curves in the plane of parameters a and b. In this contribution, we use the homotopy perturbation method to discuss the stability of Hill's equation, in particular, its transition curves. Moreover, since the homotopy analysis is not restricted to the smallness of any of its parameters, the method can determine the transition curves for large values of b.

To benchmark the accuracy of homotopy perturbation methods, we compare the analytic solution of the Meissner equation (a particular case of Hill's equation) with the obtained results from homotopy analysis. Since Hill's equation presents a periodic solution on the transition curves, transition curves with different periods do not intersect at any point. However, if two curves with the same period intersect each other, then there are two linearly independent

solutions of the same period. This last phenomenon is present in the Meissner equation, and it is interesting to discuss if the homotopy method can predict the solution in these particular points.

Koopman eigenfunction approximations by a least-squares Galerkin method

Römer, Ulrich Johannes *(Karlsruhe Institute of Technologie (KIT), Germany)* 15:50

In recent years, much attention and research has been devoted to the Koopman operator following the seminal 2005 work [1] by Mesic. The Koopman operator offers the possibility to exactly transform any dynamical system described by a (sufficiently smooth) autonomous nonlinear differential equation for its states into a (generally infinite-dimensional) decoupled linear system. More precisely, the Koopman operator is a (semi)group of linear operators with a generator that describes the so-called Kolmogorov forward equation. The time dependence of any eigenfunction φ of the Koopman operator (and its generator) is given by $d\varphi/dt = \lambda\varphi$, where λ is the corresponding eigenvalue.

Much of the current research focuses on data-driven methods for system modeling and identification, spurred by the development of dynamic mode decomposition [2] and its extensions [3] in the fluid dynamics community. These methods are algorithms for estimating eigenvalues and eigenfunctions of the Koopman operator from time series data. The core idea is a least-squares regression of ansatz functions (often referred to as a library) to map many initial states x(0) to their corresponding states x(T) after the same time interval T, resulting from the flow of the dynamical system. Often the time series data come from simulations, not measurements, and these data-driven methods are used as sophisticated post-processing methods to identify time-periodic patterns. Since the choice of appropriate ansatz functions is non-trivial, a number of extensions to the use of neural networks as universal function approximators have been investigated in recent years.

Given a system model in the form of a state-space equation and a set of ansatz functions, approximations of the Koopman eigenfunctions can also be computed using a classical Galerkin method. Since the focus of most research in Koopman operators is data-driven, this approach has not been studied as extensively. In order to compare a Galerkin approximation in terms of performance and computational effort with established data-driven methods such as (extended) dynamic mode decomposition and neural networks (in particular as autoencoders), we analyze the Koopman operator of a damped pendulum - a well-studied mechanical system whose simplicity permits interpretation of the results.

[1] Mezić, I.: Spectral properties of dynamical systems, model reduction and decompositions. Nonlinear Dynamics 41(1-3), 309-325 (2005)

[2] Schmid, P.J.: Dynamic mode decomposition of numerical and experimental data. Journal of Fluid Mechanics 65(6), 5-28 (2010)

[3] Tu, J.H. et al.: On dynamic mode decomposition: Theory and applications. Journal of Computational Dynamics 1(2), 391-421 (2014)

S05-02: Nonlinear oscillations

Date: May 31, 2023 08:30-09:30
Room: CHE/183

Nonlinear Vibrations of Bimodular Beam by Means of Isogeometric Analysis

El Chabaan, Galeb *(Technische Universität Wien, Vienna, Austria)* 08:30

The modeling and numerical analysis of dynamic response of planer rotation-free originally straight homogeneous Bernoulli-Euler beam made of bimodular materials with classical boundary conditions under time varying excitation are studied. Bimodular materials are those materials which have different elastic Young's modulus in tension and compression. In this case, the nonlinear stress-strain curve can be represented by two straight lines with slope discontinuity at the origin. This implies that the neutral axis does not pass through the geometric centroid of the cross section and depends on the curvature's sign. The change in the position of the neutral axis within a cross-section, and thus the change in the position of the centroid of stiffness during the vibration process, which describes the discontinuous behavior, can be obtained as roots of nonlinear algebraic equations, so that only one root of nonlinear equation has a physical meaning for the considered curvature. However, the position of the neutral axis depends not only on the elastic material properties but also on the geometry of the cross-section. Within this study, various symmetric trapeziodal as well as two limit cases, namely rectangular and isosceles triangular cross-sections are analyzed, showing a difference in neutral axis position between positive and negative curvatue with respect to the modular ratio. The governing equation for flexural oscilations of bimodularer beam is formulated based on model with effective two-layer laminates and discontinuous natural beam axis with respect to the axis through the cross-section's geometric centroid, that is used as an independet reference axis of the bimodular beam structure. The numerical analysis of dynamic response of the bimodular system is investigated by means of isogeometric analysis (IGA). This numerical procedure is developed to bridge the gap between computer-aided design (CAD) and finite element method (FEM). The fundamental idea behind isogeometric analysis is to use the same basis functions for constructing the exact original geometric model and for approximating the unknown solution fields. Non-Uniform Rational B-Splines (NURBS) are the most common basis functions used in the IGA. Computational application of the isogeometric finite element discretization with B-Splines to the straight Bernoulli-Euler bimodular beam is presented as a powerful tool for the analysis of bimodular structural vibrations. Finally, some numerical examples are given to verify the effectiveness of the isogeometric approach on dynamic analysis of the bimodular structures.

Detection and characterization of local nonlinearity in a clamped-clamped beam with state space realization

Gogilan, Umaaran *(Ruhr University Bochum, Germany)*
Oveisi, Atta *(Ruhr University Bochum, Germany)*
Nestorović, Tamara *(Ruhr University Bochum, Germany)*

08:50

The state space representation of linear and nonlinear systems is widely used in the literature for system characterization, system identification, and model-based control synthesis. In the case of systems with local nonlinearity, the realization of a state space model where the states are physically interpretable as a requirement has been a challenging task. This requirement becomes more emphasized, especially in the scope of industrial high-precision systems. Consequently, the class of black-box system identification approaches becomes less attractive. In the scope of this paper, we are interested in modeling systems with dominant local nonlinearity where employing linear models can only cover a limited range of system dynamics. More specifically, geometric nonlinearities which are present in the joints (bolted) of structural interfaces are analyzed. The main goal is to provide systematical modeling of such systems without using a sparse nonlinear representation. Such a low-order nonlinear model can improve the simplicity of analyzing the nonlinear system and can be used for structural vibration and noise control.

In order not to neglect the sophisticated linear modeling technique, the linear model is proposed to be extended by means of smooth nonlinear terms. The systematic approach contains the modeling of the linear counterpart followed by the localization and characterization steps in the well-known three-step paradigm. For the characterization step, this work relies on the Acceleration Surface Method (ASM).

The experimental setup under study, as a benchmark, is a set of two beams of different lengths and thicknesses connected by a screw that is excited by a mechanical shaker. The axes are oriented in the transverse direction of the beams, while the boundaries are realized as imperfect clamped-clamped boundary conditions at two ends in the model. Consequently, by selecting the excitation amplitude, we can control the dominant dynamics at lower excitation amplitudes and invoke the local nonlinearity at higher amplitudes. For higher excitation levels using sine sweep signals, the phase space information of the shaker and accelerometer sensors is used to detect the local nonlinearities along the clamped-clamped beam. The detected and characterized nonlinearities are incorporated into the linear system as a systematic approach for modeling such a structurally nonlinear system.

Various beam and shell models for nonlinear vibrations of long slender end-mills in the area of high-speed cutting

Schmidt, Rico *(TU Freiberg, Germany)*
Ams, Alfons *(TU Freiberg, Germany)*

09:10

HSC (High-Speed-Cutting) milling is an extensively used production process in tool-making and mold-making industries. For the purpose of a self-balancing tool, a hollow shaft is used and filled partially with a fluid.

This talk presents different beam and shell models for the investigation of nonlinear vibrations. Therefore, different theories are compared with respect to the influence of geometrical

nonlinearities, spin-softening as well as stress-stiffening and also shear deformation. Additionally a stochastic Wedig-Dimentberg approach is presented, for the simulation of a spatial distributed unbalance.

Starting with the nonlinear kinematics for the tool-deformation Hamilton's principle is evaluated for the variational formulation of each model. Regarding to the shear deformation the theories of Euler-Bernoulli and Timoshenko (beam models) as well as Kirchhoff-Love and Mindlin-Reissner (shell models) are used. In the following up the variational formulation is discretized under usage of a global Ritz approach on the one hand, on the other hand with a local FE-discretization. Afterwards the governing system of differential equations is solved and discussed.

Different results of rotating and nonrotating tools are presented, which show the available options of each theory and also their limits. In particular results of the eigenfrequencies including their stochastic distribution, stationary deformation, stability behavior and various time solutions are shown.

S05-03: Nonlinear oscillations

Date: June 1, 2023 08:30-10:30
Room: CHE/183

Simulation of foil bearing supported rotor systems considering tilting motions

Nitzschke, Steffen *(Otto-von-Guericke Universität Magdeburg, Germany)* 08:30
Woschke, Elmar *(Otto-von-Guericke Universität Magdeburg, Germany)*
Daniel, Christian *(Otto-von-Guericke Universität Magdeburg, Germany)*

Due to several advantages, oil free air lubricated bearings are increasingly used in rotor dynamic systems. As a consequence of the low viscosity small clearance is mandatory to ensure a reasonable load carrying capacity. In order to compensate temperature as well as centrifugal growth of shaft, the bearing shell is designed to allow elastic deformation, which is usually realised by a system of metal foils, e.g. top foil and underlying bump foil. During the design process, rotor dynamic simulations need to be carried out in order to predict vibration amplitudes due to unbalance as well as subsynchronous vibrations. The paper deals with the numerical implementation of a bump type foil bearing in a rotor dynamic simulation in order to calculate Campbell diagram and perform run-up time integration. The realised workflow utilizes an online numerical solution of the Reynolds PDE applied to ideal gas law based on FVM in combination with different models for the foil deformation, where the non-linearity of the PDE is handled with a Newton-Raphson scheme. The resulting forces carry the rotor but due to the well-known whirl excitation also cause nonlinear vibrations of the system, which occur beyond a certain rotor speed determining the stability threshold. It is state of the art to assume steady state conditions in combination with a 1d discretisation of the foil structure in the circumferential direction. The stiffness of the bump foil is often determined based on an analytical formulation or a finite element model. The paper at hand addresses an enhancement to a 2d ansatz in order to take misalignment or tilting motion of shaft into account. To describe the damping of the foil structure in an appropriate way, the time dependent foil deformation behaviour is considered, which requires inclusion of inertia properties as well as a friction model. The described formulation leads to further state space equations, which are solved by a Newmark algorithm embedded in the time integration of rotor equation of motions, where an ODE solver treats the latter. The described 2d model is compared against the usual 1d approach while they are applied to a rotor model with elastic shaft. Thus, the increase in damping due to the tilting motions to the stability limit - i.e. the occurrence of subharmonic vibrations - associated with the model extension can be evaluated in the context of the additional computational effort to be expected.

Periodic oscillations of a rotor disc in an axial flux reluctance machine

Altoé, Philipp *(Karlsruhe Institute of Technology, Germany)* 08:50
Fidlin, Alexander *(Karlsruhe Institute of Technology, Germany)*

There is increasing interest from industry in the development of new axial flux machines, as this type of electric machine promises high power density and offers an opportunity for drive

trains with little axial installation space. However, the usually disc-shaped rotors represent a rather soft structure that can easily be excited to oscillations compared to rotors in radial flux machines. In order to avoid the operation in regimes with high vibration amplitudes, the vibration behavior of the rotor under the influence of different excitations should be investigated.
In the present work, the vibration behavior of an axial flux reluctance machine is investigated using a minimal model. The rotor is modeled as a rigid disc which can tilt around a spherical joint and rotates at constant angular velocity with respect to its symmetry axis. For a fixed operating point with constant angular velocity the current excitation in the stator is assumed to be periodic in the rotation of the machine. Under this assumption, the structure of the electromagnetic forces is resulting in nonlinear restoring forces and parametric excitation for the model of the rotor disc. In addition, the rotor is subjected to unbalance excitation and/or axial excitation from a potentially coupled drive train.
The described minimal model shows periodic solutions which are studied by applying a harmonic balance method and numerical path continuation. The aim of this contribution is to point out critical operating regimes which are mainly apparent in the vicinity of parametric instabilities.

SBFEM with reduced modal basis for hydrodynamic bearings

Pfeil, Simon *(Otto von Guericke University Magdeburg, Germany)* 09:10
Song, Chongmin *(University of New South Wales, Sydney, NSW, Australia)*
Woschke, Elmar *(Otto von Guericke University Magdeburg, Germany)*

The numerical effort of transient rotordynamic simulations is often dominated by the computation of nonlinear hydrodynamic bearing forces. These forces are described by the Reynolds equation and need to be computed at every time step of the simulation. Usually, numerical models, analytical approximations, or look-up table techniques are employed, depending on the desired tradeoff between accuracy and computational cost. In recent studies, a semi-analytical approach based on the scaled boundary finite element method (SBFEM) has been developed as an efficient alternative to these methods. Along the circumferential coordinate of the bearing, a standard finite element formulation is employed, whereas in the axial direction, the solution is described analytically. A system of ordinary differential equations is obtained, leading to an eigenvalue problem. Here, the numerical effort can be further decreased by means of modal reduction, which is investigated in this study. The shaft eccentricity determines the smoothness of the hydrodynamic pressure field and is identified as an adequate indicator as to what subset of eigenvalues and eigenvectors should be considered in the solution. The developed model is incorporated into a rotordynamic simulation and compared to standard methods with respect to accuracy and efficiency.

Modeling, simulation, and implementation of a superconducting magnetic bearing twisting system in a high-speed ring spinning process

Perez Delgado, Yves Jesus *(Institute of Solid Mechanics (IFKM), Technische Universität Dresden, Dresden, Germany)*
Beitelschmidt, Michael *(Institute of Solid Mechanics (IFKM), Technische Universität Dresden, Dresden, Germany)*
Hossain, Mahmud *(Institute of Textile Machinery and High Performance Material Technology (ITM), Technische Universität Dresden, Dresden, Germany)*
Cherif, Chokri *(Institute of Textile Machinery and High Performance Material Technology (ITM), Technische Universität Dresden, Dresden, Germany)*
Abdkader, Anwar *(Institute of Textile Machinery and High Performance Material Technology (ITM), Technische Universität Dresden, Dresden, Germany)*
Baloochi, Mostafa *(Leibniz IFW Dresden, Institute for Metallic Materials, Dresden, Germany)*
Hühne, Ruben *(Leibniz IFW Dresden, Institute for Metallic Materials, Dresden, Germany)*

09:30

Ring spinning machines have been widely used for over a century in the textile industry to produce high-quality yarn, with optimum properties regarding yarn structure and tenacity, using natural or synthetic fibers. However, the conventional ring spinning process is relatively slow since it cannot be used at high spindle speeds due to the friction between the ring and the traveler which results in lower-quality yarn or the breakage of the yarn. To solve the problem, the ring/traveler system of the conventional ring spinning process was replaced with a superconducting magnetic bearing (SMB) twisting system, which consists of a permanent magnet (PM) ring and a superconductor material. The superconductor is cooled down reaching a temperature around -208°C while the PM ring is fixed with a separation between 0.5 and 2 mm. Thus, the superconductor pins the magnetic field configuration of the PM ring, resulting in a state of magnetic levitation. Due to its symmetry, the PM ring has free rotational motion concentric with the rotation of the spindle, this allows the PM ring to reach angular speeds up to 50,000 rpm. In this work, a 6-DOF dynamical model of the PM ring is obtained via the Newton-Euler equation for a rigid body, considering magnetic forces and torques that are modeled as stiffness and damping matrices. The resulting equations of motion are nonlinear, but the nonlinearity depends only on the angular speed around the main axis of rotation of the PM ring which is the z-axis. In this case, an equilibrium point exists when all the forces and torques are constant, meanwhile, the position and orientation of the PM are also constant, except for the angular speed around the z-axis which can be any constant, leading to an infinite number of equilibrium points. The linearization around any equilibrium point is performed to obtain a linear system that allows the modal analysis of the PM ring dynamics, which is important for knowing when undesirable vibrations appear. Different experiments with the SMB-ring spinning tester are performed and with the data, the unknown parameters of the model are identified. In order to validate the model, simulations are run and the results are compared with real experiments.

Acknowledgments:
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A new approach for modelling railway overhead contact lines with global shape functions to calculate dynamic contact force fluctuations

Beitelschmidt, Michael *(TU Dresden, Germany)*
Noack, Sascha *(TU Dresden, Germany)*
Hietzge, Jochen *(Institut für Bahntechnik GmbH, Dresden)*
Brandes, Enrico *(Institut für Bahntechnik GmbH, Dresden)*

09:50

The electric overhead contact line has been used for railroads for over 100 years and enables highly efficient provision of traction energy for powerful traction units. There must be reliable mechanical contact between the pantograph and the overhead contact line to ensure the transmission of electrical power without interruptions and sparking. A constant contact force at the point of contact would be ideal. The faster a train travels, the greater the dynamic effects that lead to a fluctuation in contact force. The pantograph is an oscillating system that can usually be represented sufficiently accurately by a three-mass oscillator. The catenary, on the other hand, is in complex oscillatory system that must be built from continuous and discrete model elements. The fast-moving contact between catenary and pantograph excites all involved elements to vibrate. A vibration model with associated simulation program is presented, which has been designed to specifically calculate the effects of multiple traction with several pantographs simultaneously engaged on a standard RE 200 overhead contact line. Since comparable, already existing FE models show unacceptably high computation times, a new approach was chosen here. The contact wire as well as the suspension cable are considered as strings and discretized by means of global harmonic shape functions over span lengths of up to 1000 m. Among other things, this approach has the advantage that, in contrast to FE models, there is no unphysical "sampling frequency" caused by the periodic passing of the nodes by the pantograph. Due to the design of the overhead contact line, it is necessary to provide different prestressing in the string elements in sections, which leads to a more complex calculation of the stiffness matrix. Discrete elements as well as a damping matrix can be added to the resulting mass and stiffness matrices of the strings. Overall, a linear vibration system with constant system matrices is initially obtained. The suspension cable and the catenary are coupled by the so-called hangers. The special feature of these elements is that they can buckle. These are modeled as springs acting on one side and thus represent a nonlinearity in the system. Extensive test calculations were carried out with the model, which were compared on the one hand with an FE model and on the other hand with a vibration test on a real overhead contact line. Acknowledgement: DZSF Project "Schwingungsverhalten der Oberleitung bei mehreren Stromabnehmern".

Squeak and rattle noise prediction in vehicle acoustics

Rauter, Andreas *(Technical University of Munich, Chair of Virboacoustics of Vehicles and Machines; BMW Group)*
Utzig, Lukas *(BMW Group)*
Weisheit, Konrad *(BMW Group)*
Maeder, Marcus *(Technical University of Munich, Chair of Virboacoustics of Vehicles and Machines)*
Marburg, Steffen *(Technical University of Munich, Chair of Virboacoustics of Vehicles and Machines)*

10:10

Squeak and rattle belongs to unintended noise clearly audible by occupants of a vehicle. This noise negatively affects the perceived built quality, leading to non-buying decisions, high warranty costs, and poor brand reputation. Therefore, vehicle manufacturers seek to prevent the emergence of such noise preferably in the early development phase and during production at the latest. This causes substantial monetary and temporal expenditure which must be reduced to a minimum. Rattle is defined as repeated impact. The underlying physical phenomenon is impulsive short-duration contact. Squeak in contrast originates from an in-contact motion in the tangential direction and is a friction-induced stick-slip phenomenon. State-of-the-art numerical squeak and rattle prediction is based on linear analysis resulting in an empirical noise risk index. However, quantification of noise and assessment of audibility is not possible because of non-linear contact forces and hence the actual system response is not calculable. Mathematically, the nature of both excitation events is non-linear due to frictional contact and non-smooth due to short impulsive behavior in time. This makes linear simplification and a solution process in the time domain challenging. Both events appear periodically leading to an oscillation characterized by basic and higher harmonics. Due to this periodic character, the phenomena of squeak and rattle fulfill the prerequisite for the application of the harmonic balance method (HBM) to solve the governing non-linear equation of motion. The higher the number of harmonics considered, the more precise the modeling and the dynamic response prediction are. In addition, the alternating frequency time domain method (AFT) allows switching between frequency and time domain during the iterative solution process. Thus, the non-linear contact forces can be evaluated in the time domain. The equation-solving process results in the calculation of surface velocities giving way to determining a proxy for the emitted sound power of the oscillatory system. The simulation method based on the combination of HBM and AFT was validated on test rigs for squeak and for rattle noise. The industrial applicability of this simulation approach was demonstrated numerically and experimentally on a real vehicle part showing promising results. Thereby, important steps in non-linear structural dynamics and vehicle acoustics were made toward a calm, smooth, and enjoyable ride for vehicle occupants.

S05-04: Nonlinear oscillations

Date: June 2, 2023 08:30-10:30
Room: CHE/183

Dissipation near anti-resonance in parametrically excited systems

Kraus, Zacharias *(TU Darmstadt, Germany)* 08:30
Hagedorn, Peter *(TU Darmstadt, Germany)*

The energy of linear, parametrically excited systems near anti-resonance is studied only in a few publications, focussing on illustrating the energy transfer between eigenmodes and the estimation of damping ratios. For analysis, only numerical experiments with one single initial condition were used. To gain a more profound understanding of anti-resonance, a semi-analytical approximation of the dissipated energy of each degree of freedom is derived in this contribution. The multiple scales method is used to obtain the system response, which is then averaged over the beating frequency around the difference excitation frequency. With the averaged solution, an analytical expression of the energy over time is derived. The evaluation of the expression reveals that the dissipation performance is dependent not only on the coupling terms but also on the initial energy distribution. The presented results allow for insight into the mechanisms of anti-resonance much more profound than previous approaches.

Estimation of maximum amplitude during passage through resonance

Fasih, Mohammad Saad *(Vorarlberg University of Applied Sciences, Austria; UMIT TIrol – Private University for Health Sciences and Health Technology)* 08:50
Dohnal, Fadi *(Vorarlberg University of Applied Sciences, Austria)*

The main motivation for developing this procedure is to extract an analytical estimation for the maximum vibration response during passage through resonance. The homotopy analysis method (HAM) is a semi-analytical technique that can be applied to find approximate solutions of nonlinear systems described by ordinary differential equations. In contrast to perturbation techniques, the method does not need an artificially small parameter for guaranteeing convergence. We apply HAM to develop an analytical approximation of the maximum amplitude of a linear oscillator during passage through resonance. Approximations derived by different methodologies exist in the literature and are valid within specific regions of system parameters. The current results are benchmarked against existing approximations.

Numerical detection of synchronisation phenomena in quasi-periodic solutions

Seifert, Alexander *(University of Kassel, Germany)* 09:10
Bäuerle, Simon *(University of Kassel, Germany)*
Hetzler, Hartmut *(University of Kassel, Germany)*

In science and technology, dynamical systems can show so called quasi-periodic solutions. These solutions contain two or more so-called base frequencies. Base frequencies are characterised by the fact that their ratio to each other is an irrational number. This leads to the solution no longer being periodic, while retaining a discrete frequency spectrum. A quasi-

periodic solution trajectory is densely embedded on a torus manifold by which it can alternatively be represented. For the parameterisation of such torus solutions, the Hyper-Time-Approach is suitable. This parametrisation approach leads to a system of partial differential equations describing the torus surface. An important restriction is that the Hyper-Time-Approach is only valid, as long as the number of base frequencies remains unchanged. If quasi-periodic solution branches are continued, the effect of synchronisation may occur, in which the number of base frequencies reduces. The simplest example is a quasi-periodic solution with two base frequencies, in which the two occurring frequencies synchronise, i.e. in a Neimark-Sacker bifurcation, and a periodic solution results. As an academic example, we consider the externally excited van der Pol system, which shows periodic and quasi-periodic solutions. The mechanism of "suppression of the natural dynamics" (suppression), in which the amplitude of the self-excitation frequency disappears, is one possible scenario how synchronisation may occur. This corresponds to a contraction of the torus until a periodic solution remains, when passing through the synchronisation point. The mechanism of suppression is accompanied by the occurrence of a Neimark-Sacker bifurcation. The detection of a Neimark-Sacker bifurcation, on a periodic solution branch can be performed by means of test functions known from literature. Such a test function typically marks a bifurcation point by a sign change. It is often based on stability information of the periodic solution. The main challenge is to derive a test function, with which Neimark-Sacker bifurcations can be detected based on a quasi-periodic solution. Additionally, since the Hyper-Time-Approach only applies up to the synchronisation point, a sign-changing test function cannot be derived. Instead, we derive a function that becomes zero at the synchronisation point and detect an approach of this zero up to a given tolerance. Therefore, we synthesise Poincaré sections from the Hyper-Time manifold and investigate the evolution of the averaged cross-sectional area of these Poincaré sections. This allows us to detect the synchronisation of quasi-periodic solutions, due to suppression by using the Hyper-Time-Approach.

Critical Manifolds in a Simple Two-wheel Vehicle Model

Steindl, Alois *(TU Wien, Austria)*
Edelmann, Johannes *(TU Wien, Austria)*
Plöchl, Manfred *(TU Wien, Austria)*

09:30

We consider a simple two-wheel vehicle model, assuming a brush model for the tyre behaviour. In recent numerical investigations of the vehicle dynamics we frequently observed singular perturbation phenomena, like Canard explosions and periodic solutions with large periods, which evolve along slow manifolds for a long time. These situations occur, when both the front and rear wheel operate in their saturation regimes. In this talk we intend to explain the observed behaviour using the methods of geometric singular perturbation theory. We determine the singular and slow manifolds and study their stability properties.

Continuation and stability analysis of quasi-periodic solution branches: A unified framework based on different torus discretization strategies

Bäuerle, Simon *(University of Kassel - Institute for Mechanics - Engineering Dynamics, Germany)*
Seifert, Alexander *(University of Kassel - Institute for Mechanics - Engineering Dynamics, Germany)*
Kappauf, Jonas *(University of Kassel - Institute for Mechanics - Engineering Dynamics, Germany)*
Hetzler, Hartmut *(University of Kassel - Institute for Mechanics - Engineering Dynamics, Germany)*

09:50

We present a framework for continuing stationary solution branches and conducting stability analysis in dynamical systems. Our approach enables the computation of equilibria, periodic orbits and two-fold quasi-periodic tori by using and combining different discretization methods. In dynamical systems, stationary solutions or limit sets are of significant interest to researchers and practitioners. In recent years, quasi-periodic oscillations have gained importance in application-oriented research. These oscillations are a type of *higher order* periodic solution: their Fourier transforms contain at least two fundamental frequencies (and corresponding higher harmonics) that have no rational ratio (e.g., 1 and π). This leads to an infinite period length. Furthermore, the quasi-periodic trajectory lies on a two- (or higher-) dimensional torus in state space. It follows from the infinite period length that the trajectory densely fills the torus hyper-surface (manifold). Thus, it is permissible to study the finite surface instead of the infinite trajectory. These tori can be computed using different approximation schemes to solve the underlying partial differential equations. However, usually a whole family of solutions, a so-called branch, is of interest instead of a single solution. A common method for efficient computation of such branches are predictor-corrector schemes. Several powerful software codes, such as MatCont, NLVib, and MANLab, are available for these tasks in Matlab. These toolboxes are primarily based on a single discretization scheme for periodic orbits or quasi-periodic hypersurfaces. Based on our previous research on different discretization methods, we are working on an alternative toolbox for the continuation of equilibria, periodic orbits as well as quasi-periodic hypersurfaces. The core architecture combines various elements of the three toolboxes mentioned above. The main difference is the possibility to deliberately chose different discretization schemes such as finite differences, (multi-)harmonic balance or multiple shooting methods depending on the problem. The framework also allows easy incorporation of further methods. Additionally, the toolbox enables the determination of the (Lyapunov) stability of equilibria, periodic and quasi-periodic solutions by computing eigenvalues, Floquet multipliers or Lyapunov exponents. In this contribution, we provide a brief overview of existing toolboxes and introduce our proposed framework. We also compare two different methods for discretizing quasi-periodic hypersurfaces using the example of a quasi-periodically forced Duffing oscillator.

Stability analysis of roller coaster trains along spatial trajectories

Zamora Agustí, Marc Guillem *(Universität Duisburg-Essen, Germany)*
Kecskeméthy, Andrés *(Universität Duisburg-Essen, Germany)*
10:10

It is well known that vibrations usually appear during a roller coaster ride, which in some cases leads to passenger discomfort and poses additional material and structural strain. However, the causes of such vibrations are still not fully understood. While there have been technological advances that help to mitigate them to some degree, for instance by placing shock absorbers between the wheels and the bogie frame, an analysis of this phenomenon is required to make better decisions at the design stage. A few multibody simulation approaches have been proposed in the literature, including simplified train structures with lumped mass elements and wheel-rail compliant contact models. In a previous work, a mismatch between simulated spatial frequencies and real measurements was found out, potentially indicating disregarded phenomena. A novel model is proposed to this end, which describes the complete kinematic tree separating the overall spatial trajectory motion from the relative motions between train components, and expresses the contact problem in terms of the trajectories of an ideal system solved a priori. This approach reduces the computational complexity whilst preserving a flexible description of the contact forces, here extended with respect to previous works by considering additional creep forces at the wheel-rail contact interface. Due to the rapidly changing configuration of a roller coaster train, classical stability analysis may only be used in singular cases, for instance during a horizontal banked curve at a constant speed. Instead, transient stability indicators are proposed, based on the response of the system starting at arbitrary track locations after an initial perturbation. Without the presence of external excitations, that is, trajectory deviations or local defects, various regions of instability are detected, thus indicating a possible self-excitation in real systems. This approach can also be extended to account for perturbations of the precomputed ideal system.

S06.1: Material modelling with metals

Organizer(s): **Mosler, Jörn** *(TU Dortmund)*
Kurzeja, Patrick *(TU Dortmund)*

S06.1-01: Material modelling with metals

Date: May 31, 2023 14:00-16:00
Room: POT/112

A variational approach for the cyclic behavior of nickel titanium under thermal as well as mechanical loading

Waimann, Johanna *(RWTH Aachen University, Germany)* 14:00
Junker, Philipp *(Leibniz Universität Hannover, Germany)*

Thermally as well as mechanically induced solid/solid phase transformations between austenite and martensite are the reason for the special properties of nickel titanium, such as the superelasticity and the shape memory effect. However, due to interactions with other microstructural effects like dislocation formation and movement, the phase transition is influenced. Especially during cyclic loading one can detect the effect of functional fatigue [1] which limits the material's predictability and thus its industrial applicability. We present a variational method to take into account the cyclic behavior of this special class of materials, including inelastic effects such as the formation of a remaining strain and the influence on the changing start of the phase transformations. Compared to our earlier works, e.g. [2], the model accounts for both thermally as well as mechanically induced cycling and related fatigue effects. To consider the polycrystalline structure of the metal alloy, we use an evolving averaged orientation of the transforming grains provided by [3]. The presentation is completed by numerical results to show the approach's functionality and to compare it with experimental findings.

[1] G. Eggeler, E. Hornbogen, A. Yawny, A. Heckmann and M. Wagner: Structural and functional fatigue of NiTi shape memory alloys. *Materials Science and Engineering: A*, *378*(1-2), 24-33 (2004).
[2] J. Waimann, K. Hackl and P. Junker: Variational modeling and finite-element simulation of functional fatigue in polycrystalline shape memory alloys. *Journal of Optimization Theory and Applications*, *184*, 98-124 (2020).
[3] P. Junker: A novel approach to representative orientation distribution functions for modeling and simulation of polycrystalline shape memory alloys. *International Journal for Numerical Methods in Engineering*, *98*(11), 799-818 (2014).

Applying the Simplified Theory of Plastic Zones to Single-Parameter Cyclic Loading

Zobel, Maximilian *(BTU Cottbus-Senftenberg, Germany)* 14:20
Hübel, Hartwig *(BTU Cottbus-Senftenberg, Germany)*
Vollrath, Bastian *(BTU Cottbus-Senftenberg, Germany)*
Dornisch, Wolfgang *(BTU Cottbus-Senftenberg, Germany)*

The asymptotic behaviour of components under cyclic over-elastic loading basically falls into one of three categories: The unlimited increase of strains (ratcheting or incremental collapse),

a cyclic opposite increase and decrease of elastic-plastic strains associated with a limited accumulation of strain (plastic shakedown or cyclic/alternating plasticity) or the accumulation of elastic-plastic strain associated with pure elastic strain ranges (elastic shakedown). The Simplified Theory of Plastic Zones (STPZ) is a direct method for predicting the behaviour of structures subjected to cyclic loading, thus avoiding a step-by-step analysis of the entire load history to obtain the range and the accumulation of elastic-plastic strains in the shakedown state. In this talk the fundamentals of the STPZ will be presented, in regard to single-parameter cyclic loading and unlimited kinematic hardening. Finally, the results of the STPZ applied to an example will be compared to a step-by-step analysis.

The simulation of residual stress evolution during cyclic loading

Schneider, Tom *(Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany)*
Kästner, Markus *(Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany)*
14:40

Residual stresses can have a major impact on the performance of a metallic component under cyclic loading. Understanding the magnitude, occurrence, and behavior of residual stresses under such loading could improve the way engineering structures are designed and manufactured. In particular, compressive residual stresses are beneficial in terms of increasing fatigue life. However, this is only true if the residual stresses remain in the structure over the fatigue life, which necessitates the study of the evolution of residual stresses under cyclic load.

In the talk, an experimental setup is presented in order to study the formation and cyclic evolution of residual stresses. The experiments are accompanied by simulations to show relevant issues when it comes to modelling residual stress evolution. Since a pure bending state is the simplest way to induce residual stresses by forming, four-point bending specimens are used. They undergo cyclic deformation which leads to change in residual stresses with respect to the initial state after the first loading. Over fatigue life, the experiment is stopped at various load cycles and the specimens are used for the experimental measurement of the residual stress state. Afterwards, the experimental results are compared to the simulation of the cyclic residual stress evolution. For this example of bending specimens, special emphasis is put on the plasticity model framework and the impact of this choice on the simulations result. The parameterization and application of a plasticity model capable of capturing fundamental effects of cyclic plasticity is shown and compared to experimental data obtained on the cyclic bending tests. It is presented that the modelling of residual stress evolution is a challenging task which must be critically evaluated regarding the model choice and parametrization.

Characterisation of damage by means of electrical measurements: numerical predictions

Güzel, Dilek *(TU Dortmund, Germany)*
Kaiser, Tobias *(TU Dortmund, Germany)*
Menzel, Andreas *(TU Dortmund, Germany; Lund University, Sweden)*

15:00

Ferrite/martensite dual-phase (DP) steels have been the focus of research and industrial applications over the past decades. DP steels are attractive materials for automotive-related sheet forming applications since they have high ultimate tensile strength, high ductility, and macroscopically homogenous plastic flow. These property enhancements are achieved by ferritic and martensitic constituents. However, the combination of ferritic and martensitic constituents also leads to the nucleations of voids, martensite cracking, and decohesion of phase or grain boundaries due to the strong contrast of the constituents when undergoing plastic deformations [1]. Therefore, understanding the damage mechanisms and quantifying the damage is important to optimise structures and increase their reliability. To achieve this goal, experimental- and simulation-based techniques are to be combined.

Different methods exist for the analysis of damage phenomena, such as fracture mechanics, phase field models, cohesive zone formulations and continuum damage modelling. Assuming a typical [1 − d]-type damage formulation, the governing equations of continua that account for damage under mechanical and electrical loads are derived. The mechanical and electrical subproblems give rise to the local form of the balance equation of linear momentum and the continuity equation for the electric charge, respectively. Experimental investigations indicate that changes in electrical conductivity can arise due to the underlying microstructure, e.g. cracks [2] or dislocations [3]. Therefore, motivated by deformation-induced property changes, the effective electrical conductivity is assumed to be a function of the damage variable. This eventually allows the prediction of experimentally recorded changes in the electrical resistance due to mechanically-induced damage processes. Interpreting the resistivity as a fingerprint of the material microstructure, the simulation approach proposed in the present work contributes to the development of non-destructive electrical-resistance based characterisation methods. To demonstrate the applicability of the proposed framework, different representative simulations are studied. The measured changes in resistance due to damage are compared against numerical predictions.

[1] R. Meya, C. F. Kusche, C. Löbbe, T. Al-Samman, S. Korte-Kerzel, and A. E. Tekkaya, “Global and high-resolution damage quantification in dual-phase steel bending samples with varying stress states,” Metals, vol. 9, p. 319, 2019.
[2] M. J. Cordill, O. Glushko, and B. Putz, “Electro-mechanical testing of conductive materials used in flexible electronics,” Front. Mater., vol. 3, p. 11, 2016.
[3] H. Bishara, H. Tsybenko, S. Nandy, Q. K. Muhammad, T. Frömling, X. Fang, J. P. Best, and G. Dehm, “Dislocation-enhanced electrical conductivity in rutile tio2 accessed by room-temperature nanoindentation,” Scr. Mater., vol. 212, p. 114543, 2022.

Isogeometric Analysis for Sintering Hollow Spheres

Wiegold, Tillmann *(Technische Universität Dortmund, Germany)*
Kurzeja, Patrick *(Technische Universität Dortmund, Germany)*
Mosler, Jörn *(Technische Universität Dortmund, Germany)*
15:20

The current presentation deals with the simulation of sintering of hollow spheres. Hollow sphere structures enable a high stiffness to weight ratio. An accurate prediction of their properties is hence relevant, for instance, for light-weight construction [1, 2]. The focus of the present analysis is placed on the initial stages of the sintering process, during which spheres connect by neck bridging. Starting from an initial contact point between two adjacent spheres, the sintering process itself is characterized by the size of the contact area evolving from this point. It is driven by various diffusion mechanisms, for example, surface-dominated or bulk-dominated diffusion [3]. The final orientation and deformation of the spheres are then determined in combination with the underlying mechanical problem, e.g., under additional compression of the assembly. The significant smaller wall thickness compared to the diameter moreover motivates a simplification of spheres as 2D shell objects in a 3D environment. The present work applies isogeometric analysis (IGA) for the simulation of the sintered spheres, which strongly benefits from the spherical geometry. Furthermore, IGA provides higher order derivatives of the shape functions [4] enabling a natural incorporation of curvature effects. The generated spheres are geometric exact and C1-continuous at every point. The presented framework moreover allows to account for various diffusion mechanisms such as grain boundary diffusion or surface diffusion, driving the development of the contact area. Selected numerical example illustrate the sintering behaviour of different configurations of spheres and their mechanical response.

References:

[1] O. Andersen, U. Waag, L. Schneider, G. Stephani and B. Kieback. https://doi.org/10.1002/(SICI)1527-2648(200004)2:4%3C192::AID-ADEM192%3E3.0.CO;2-%23

[2] A. Kennedy https://doi.org/10.5772/33060

[3] D. Pino-Munoz, J. Bruchon, S. Drapier and F. Valdivieso. https://doi.org/10.1007/s11831-014-9101-4

[4] Piegl, Les, and Wayne Tiller. The NURBS book. Springer Science & Business Media, 1996.

Coupled strain and temperature gradient analysis in curved surfaces

Müller-Lohse, Lutz *(TU Clausthal, Germany)*
Tröger, Jendrik-Alexander *(TU Clausthal, Germany)*
Hartmann, Stefan *(TU Clausthal, Germany)*
15:40

A common method in experimental mechanics is 3D Digital Image Correlation (DIC) for determining deformations of curved surfaces, whereby the motion of material points is measured. The temperatures induced by the deformation of surfaces due to dissipative effects are of particular interest. In this context, surface temperatures can be measured using infrared thermography systems. However, the disadvantage of this approach is that a thermographic camera only provides the two-dimensional temperature distribution of three-dimensionally curved surfaces (plane images). Thus, temperature gradients cannot be specified. However,

for most problems the temperature and the motion of material points are of particular interest. In the literature, planar problems are studied and simplifying assumptions are made so that a simple coupling of thermography and DIC is possible. In contrast, this contribution presents a method where 3D DIC is coupled with thermography in such a way that the temperature, temperature gradient, as well as displacement and strain distributions at material points of curved surfaces can be determined over time. The method also allows a continuous strain and temperature gradient determination over the entire domain, since a special class of functions named Radial Basis Functions is used for interpolating the measured data.

S06.1-02: Material modelling with metals

Date: June 1, 2023 08:30-10:30
Room: POT/112

Constitutive modeling of single and oligo crystals based on an Augmented Lagrangian formulation – Application to TWIP-steels and SMAs

Prüger, Stefan *(Technische Universität Bergakademie Freiberg, Germany)* 08:30
Löps, Paul *(Technische Universität Bergakademie Freiberg, Germany)*
von Oertzen, Vincent *(Technische Universität Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(Technische Universität Bergakademie Freiberg, Germany)*

Multi-scale modeling of polycrystalline materials has gained considerably attention over the last decades due the availability of high performance computing capabilities and efficient numerical algorithms, e.g. FFT- and FE^2-schemes. Although such an approach intrinsically provides the effective constitutive response of the material on the polycrystal scale, it crucially depends on the choice of a physically sound material model and its numerically robust implementation at the single crystal scale. Constitutive relations of single crystals typically incorporate finite deformations and must account for anisotropy effects, stemming both from anisotropic elasticity and the restriction of inelastic deformations to a set of discrete slip- and transformation systems. To robustly determine the set of active systems is challenging, particularly in the rate-independent case, for which the problem is ill-posed. However, an Augmented Lagrangian formulation of the principle of maximum dissipation proved to be very robust in this regard, when applied to a model for cubic single crystals with different degrees of anisotropic hardening [1].
Within the current contribution, such an approach is applied to the modeling of miniaturized tensile tests, showing an oligo-crystalline microstructure. Model predictions are compared in depth to experimental results, involving measurements from Electron Back-Scatter Diffraction and Digital Image Correlation. Furthermore, an extended Augmented Lagrangian formulation is presented that accounts for bound constraints on internal state variables, e.g. required for the constituent volume fractions in a phase transforming material. The single crystal model for NiTi-shape memory alloys, described in [2], is adopted to assess the performance of the Augmented Lagrangian solution algorithm. Moreover, the model formulation is generalized to capture the characteristic responses of iron-based SMAs.

[1] S.Prüger, B.Kiefer, Int. J. Mech. Sci., 180, pp.105740, 2020
[2] L.Anand, M.E.Gurtin, J. Mech. Phys. Solids, 51(6), pp.1015–1058, 2003

On the numerical efficiency and robustness of interior-point algorithms for finite strain rate-independent single crystal plasticity

Niehüser, Alexander *(Institute of Mechanics, TU Dortmund University, Germany)* 08:50
Mosler, Jörn *(Institute of Mechanics, TU Dortmund University, Germany)*

Crystal plasticity models incorporate crystallographic slip systems into the constitutive model and offer a powerful framework for analyzing plasticity at the micro- as well as the macroscale. However, classical rate-independent crystal plasticity models face long standing problems regarding activity and linear dependence of slip systems leading to non-unique solutions. Most solution strategies for the aforementioned problems rely on an heuristic active set search in

combination with a numeric manipulation of the linear system of equations. However, when crystal plasticity is recast as a constrained optimization problem, it is suitable for optimization schemes such as the augmented Lagrangian approach or interior-point formulations. The latter has recently been applied but a discussion on important algorithmic features and properties is still pending. This is precisely the focus of this work. To be more precise, the choice of suitable solution strategies and algorithmic parameters to develop an efficient and robust algorithm are discussed. Furthermore, well-posedness of the resulting algorithm is analyzed and different concepts for treating the singular algorithmic consistent tangent modulus are reviewed. The robustness and efficiency of the final algorithm are compared to the augmented Lagrangian formulation by means of several numerical examples.

A modular data-driven approach for inelasticity based on history surrogates

Bartel, Thorsten *(Institute of Mechanics, Technical University Dortmund, Germany)* 09:10
Harnisch, Marius *(Institute of Mechanics, Technical University Dortmund, Germany)*
Schweizer, Ben *(Chair I (Analysis), Technical University Dortmund, Germany)*
Menzel, Andreas *(Institute of Mechanics, Technical University Dortmund, Germany; Division of Solid Mechanics, Lund University, Sweden)*

The data-driven mechanics, introduced in 2016 by Kirchdoerfer and Ortiz, is a method in the field of computational mechanics, which replaces conventional material models with data sets containing matching pairs of stresses and strains. The solution of the boundary value problem is based on minimizing a distance between states within these data sets, referred to as material states, and states satisfying equilibrium conditions and kinematic compatibility, referred to as mechanical states. Current research in this area addresses the challenging task of extending the method to account for path-dependent material behavior. In this contribution, we present a novel approach to tackle this task by the extension in terms of two quantities: A history surrogate, that stores essential information on the history of the material up to the current point in time and an associated propagator that serves as an update rule.

One distinctive feature of our approach is that these quantities are used as substitutable modules that affect both data generation and data-driven simulation. In detail, the framework consists of six modules: The first one is defined by the raw input data, i.e. the paths of discrete stress-strain pairs which contain the information of the materials behavior to be depicted. The suitable history surrogate is defined in the second module and updated via the propagator, representing the third module. Both previous modules are utilized in the fourth module to construct a data set. The data-driven solver, being the fifth module, uses this data set to calculate a physically admissible solution to the given boundary value problem. The search algorithm for the determination of the current material states represents the sixth module. Due to this modularity, the structure of the original approach is maintained, thereby allowing for a straightforward extension of existing codes for elasticity.

In addition to the possibility of an intuitive definition, which may only apply to specific cases, a universally applicable approach is a Neural Network as history surrogate and propagator. The resulting framework is able to find a suitable history surrogate and to perform data-driven simulations of inelastic material behavior solely based on the raw input data. On this basis,

we highlight the capabilities of our novel approach by presenting results of different inelastic processes, e.g. plasticity and phase transformations in shape memory alloys, different non-monotonic loading paths, and different solvers, e.g. a staggered and a MIQP solver.

Finite element modeling of the phase transformation behavior in metastable austentic stainless steels

Thammineni, Hari Kisan *(Institute for Mechanics, Technical University of Darmstadt, Franzika-Braun-Straße 7, 64287-Darmstadt, Germany.)*
Denzer, Ralf *(Division of Solid Mechanics, Lund University, Ole Römersväg 1, 22100-Lund, Sweden.)*
Hallberg, Håkan *(Division of Solid Mechanics, Lund University, Ole Römersväg 1, 22100-Lund, Sweden.)*
Müller, Ralf *(Institute for Mechanics, Technical University of Darmstadt, Franzika-Braun-Straße 7, 64287-Darmstadt, Germany.)*
09:30

The transformation from the austenitic phase to the martensitic phase due to the applied plastic strains, observed in metastable Cr-Ni steels is simulated. Plastic flow behavior in the individual phases is modeled using viscoplastic power law type equations. The shear strengths of austenite and martensite used in these equations also evolve with the plastic strains in their respective phases. The macroscopic stress-strain response is then computed by an analytical homogenization method. The phase transformation process is considered to be dependent both on plastic strain in the austenitic phase and the stress state. The model is implemented using finite strain continuum mechanical formulations and is solved using implicit time integration. Using least-squares optimization the material parameters in the model are estimated by fitting with the experimental data. The model is then tested on a few structured boundary value problems.

Recovery of Battery Ageing Dynamics using Bayesian Inference

Selahi, Alireza *(WIAS, Germany)*
09:50

Rechargeable batteries play an important role in our modern society, with application ranging from smartphones over medical devices to electric vehicles or even battery plants. Lithium ion based batteries (LIBs) are yet the dominant technological standard and were honored by the 2019 Nobel Prize in Chemistry. However, LIBs suffer from different degradation phenomena. Based on a modeling framework developed by Landstorfer et al., we model degradation phenomenologically by assuming that the diffusivity of the Lithium-ions decreases with each charge-discharge cycle. Given data sets of these cycles, the challenge is to identify the evolution behavior of the diffusivity. This is an inverse problem. In this work, we employ modern methods of Bayesian inference to tackle this inverse problem and to identify the parameters of this degradation.

Automating constitutive modeling by Machine Learning: a lightweight ML approach for cyclic plasticity

Hildebrand, Stefan *(Department of Structural Mechanics and Analysis, TU Berlin, Germany)*
Klinge, Sandra *(Department of Structural Mechanics and Analysis, TU Berlin, Germany)*

10:10

Machine Learning (ML) methods are more and more involved in material modeling with the goal to replace analytical constitutive models by machine-learned relationships. Apart from the possible simplification of existing approaches, the application of ML is motivated by the increasing automatization of material characterization. The present talk particularly focuses on modeling of cyclic plasticity which is crucial for an accurate fatigue analysis.

The model proposed assumes von Mises flow rule and the associated plasticity framework as a basis. Moreover, it uses pseudo-experimental data and lightweight Feed Forward Neural Networks to completely replace assumptions on the mixed kinematic and isotropic hardening. The approach is strongly motivated by the fact that the existing analytical assumptions even with the introduction of several internal hardening parameters [1] are only partially able to represent the complex stress-strain dependency typical of realistic cyclic behavior.

The numerical investigations performed with different network architectures indicate that a direct training of a six-dimensional stress tensor is not feasible and show that the reduction of the problem complexity is key for a successful training and a low generalization error. This has been achieved by learning the plastic multiplier and the evolution of backstresses. The training data set is generated by random walks constructed by Gaussian Processes. An optimal lightweight architecture is determined by systematically varying the number of hidden layers, neurons and activation functions. In terms of computational effort necessary for training and prediction, the final configuration has shown a significant improvement compared to the alternative approaches based on the application of Recurrent Neural Networks. The validation of the model has been performed on the example of dual-phase steels.

[1] - S. Aygün, T. Wiegold and S. Klinge. Coupling of the phase field approach to the Armstrong-Frederick model for the simulation of ductile damage under cyclic load. *Int. J. Plast.*, 143:103021, 2021.

S06.1-03: Material modelling with metals

Date: June 2, 2023 08:30-10:30
Room: POT/112

Implementation of crystal plasticity in the context of multiphase-field method and jump conditions

Prahs, Andreas *(Institute for Applied Materials - Microstructure Modelling and Simulation (IAM-MMS), Karlsruhe Institute of Technology (KIT))*
Schöller, Lukas *(Institute for Applied Materials - Microstructure Modelling and Simulation (IAM-MMS), Karlsruhe Institute of Technology (KIT); Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Sciences)*
Schneider, Daniel *(Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Sciences; Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT))*
Nestler, Britta *(Institute for Applied Materials - Microstructure Modelling and Simulation (IAM-MMS), Karlsruhe Institute of Technology (KIT); Institute of Digital Materials Science (IDM), Karlsruhe University of Applied Sciences; Institute of Nanotechnology (INT), Karlsruhe Institute of Technology (KIT))*

08:30

Regarding the investigation of the plastic material behavior of polycrstalline materials, simulation studies and experimentally determined characteristics are commonly compared with respect to a wide range of scales. The crystalline microstructure, such as the slip systems of an underlying crystal lattice, are taken into account by the crystal plasticity theory (CP), cf., e.g., [1]. Describing the plastic deformation entirely in terms of the plastic slip, the CP represents a phenomenological theory. However, in contrast to methods that explicitly account for fundamental mechanisms, it offers the possibility to compare experimental results with simulations up to specimen size, cf., e.g., [2]. In classical continuum mechanics, grain boundaries are commonly represented by material singular surfaces and, thus, as sharp interfaces between neighbouring grains, cf., e.g., [3]. The tracking of these sharp interfaces is numerically costly, especially if an evolving polycrstalline microstructure is considered. The implementation of the CP in the context of the multiphase-field method (MPFM) provides a numericaly efficient method for treating moving interfaces. In MPFM, interfaces are treated in a smeared out way as diffuse regions of finite thickness. With respect to the implementation of the constitutive material behavior in the diffuse interface region, the possibilities discussed in literature can essentially be assigned to three approaches: Interpolation, homogenization, and jump condition approaches. The jump condition approach, cf., e.g., [5], [6], fulfills the balance of linear momentum for a material singular surface as well as the Hadamard condition. Here, the implementation of the classical CP within the MPFM by means of the jump condition approach is presented. Three dimensional simulations of a bicrystal are considered for a comparison of the jump condition approach and the interpolation approach. The application to multliple phases is illustrated by simulations regarding a periodic honeycomb structure as well as a grain aggregate of eight differently oriented grains.

References

[1] R. J. Asaro, J. Appl. Mech., Vol. 50 (4b), 921-934, 1983.
[2] E. Bayerschen, A. Prahs, S. Wulfinghoff, M. Ziemann, P. A. Gruber, M. Walter, T. Böhlke, J.

Mater. Sci., Vol. 51 (16), 7451-7470, 2016.
[3] A. Prahs, T. Böhlke, Contin. Mech. Thermodyn, Vol. 32, 1417-1434, 2019.
[4] J.R. Willis, Adv. Appl. Mech., Vol. 21, 1-78, 1981.
[5] J. Mosler, O. Shchyglo, H. Montazer Hojjat, J Mech Phys Solids, Vol. 68, 251-266, 2014.
[6] D. Schneider, F. Schwab. E. Schoof, A. Reiter, C. Herrmann, M. Selzer, T. Böhlke, B. Nestler, Comput. Mech., Vol. 60 (2), 203-217, 2017.

Investigation of microstructure evolution accounting for crystal plasticity in the multiphase-field method

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Prahs, Andreas *(Institute for Applied Materials - MMS, Karlsruhe Institute of Technology (KIT))*
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08:50

Regarding microstructured materials, a quantitative prediction of phase transformation processes is highly desirable for a wide range of applications. With respect to polycrstalline materials, the plastic material behavior is commonly investigated using a crystal plasticity (CP) theory [1], since it accounts for the underlying microstructure, i.e., slip systems of the crystal lattice. In classical continuum mechanics, grain boundaries (GBs) are commonly modeled as material singular surfaces, cf., e.g., [2]. However, the tracking of moving GBs, present during phase transformation processes, is numerically challenging and costly. This can be circumvented by the incorporation of CP within the multiphase-field method (MPFM), which provides a numerically highly efficient method for the treatment of moving interfaces, considered as diffuse interfaces of finite thickness.

In this work, the implementation of the constitutive material behavior within the diffuse interface region accounts for phase-specific plastic fields, cf., e.g., [3] and the jump condition approach, cf., e.g., [4, 5, 6]. The microstructure evolution and growth of inclusion is investigated within the MPFM accounting for CP. To improve the understanding of the impact of a driving force arising from plastic deformation on the phase evolution, a single inclusion problem is analyzed. In this setup, the plastic deformation of the matrix arises from eigenstrains applied to the purely elastic inclusion. The phase evolution is conducted until an equilibrium of the contributions to the total driving force is reached. The resulting equilibrium shapes are illustrated and examined. Further investigations are inspired by the principles of recrystallization. For this purpose, the phase evolution of an elastic and undeformed nucleus within

a highly deformed region is investigated. In this framework the impact of the plastic driving force can be analyzed separately.

References:
[1] R. J. Asaro, J. Appl. Mech., Vol. 50 (4b), 921-934, 1983.
[2] A. Prahs, T. Böhlke, Contin. Mech. Thermodyn, Vol. 32, 1417-1434, 2019.
[3] C. Herrmann, E. Schoof, D. Schneider, F. Schwab, A. Reiter, M. Selzer, B., Nestler, Comput. Mech., Vol. 62, 1399-1412, 2018.
[4] A. Durga, P. Wollants, N. Moelans, Model. Simul. Mater. Sci. Eng., Vol. 21 (5), 055018, 2013.
[5] J. Mosler, O. Shchyglo, H. Montazer Hojjat, J Mech Phys Solids, Vol. 68, 251-266, 2014.
[6] D. Schneider, F. Schwab. E. Schoof, A. Reiter, C. Herrmann, M. Selzer, T. Böhlke, B. Nestler, Comput. Mech., Vol. 60 (2), 203-217, 2017.

Phase field modelling of thermo-mechanical fatigue damage in Ni-based superalloys

Gao, Hanghang *(RWTH Aachen University, Germany)* 09:10
Ma, Songyun *(RWTH Aachen University, Germany)*
Markert, Bernd *(RWTH Aachen University, Germany)*

Nickel-based superalloys are widely used in aircraft engines and nuclear reactors due to their excellent creep-fatigue resistance. The complex thermo-mechanical damage process of Ni-based superalloys under service conditions is associated with different physical mechanisms. Therefore, quantifying their fatigue behaviour is still challenging for designing long-term reliable components. To this end, the phase field method has recently emerged as a promising approach to predict thermo-mechanical fatigue damage evolution, and simulate fatigue crack growth in a multiphysics context. This work presents an approach to describe the thermo-mechanical fatigue (TMF) damage behaviour of nickel-base superalloys using the phase field method, which is coupled with an elastoviscoplastic model within the thermodynamic framework. The phase field model naturally accounts for the coupling of heat transfer, inelastic deformation and fatigue fracture in the TMF process. The variational formulation used ensures consistency with the laws of thermodynamics. The results show that the proposed model can predict nickel-base superalloys' fatigue lifetime and damage evolution under thermal cyclic loading conditions. The proposed model provides a novel approach for evaluating the TMF performance of nickel-base superalloys.

Phase-field investigations of new low-order explicit last stage diagonal implicit Runge-Kutta schemes (ELDIRK) with the finite-element method

Westermann, Hendrik *(Paderborn University, Germany)* 09:30
Mahnken, Rolf *(Paderborn University, Germany)*

Runge-Kutta algorithms with adaptive step size control provide suitable tools for the solution of initial value problems (IVP). To estimate the error of the embedded scheme in the established Runge-Kutta-Fehlberg methods, only one more function calculation is necessary. The disadvantage to Fehlberg's approach is the fully explicit nature of the schemes. To conquer the remedy of the explicit downsides, diagonal implicit Runge-Kutta schemes (DIRK) are applied, employing a semi-implicit approach. Since these methods miss the advantage

of Fehlbergs idea, to obtain an error estimate with only one additional function evaluation, DIRK are generally not suited for embedded algorithms. The same holds for the explicit diagonal implicit Runge-Kutta approach (EDIRK). This work presents a general approach for the construction of new low-order Runge-Kutta methods by combining implicit schemes with the above-mentioned additional explicit evaluation as an explicit last stage. This results in Butcher tableaus with two solutions of different orders of convergence suitable for embedded methods, where additional explicit evaluations achieve the higher-order solution. Thus, the iterative solution of non-linear systems is omitted for the additional stage, presenting a major reduction in computational cost. Embedded Butcher tableaus for the novel explicit last stage diagonal implicit Runge-Kutta schemes (ELDIRK) are presented for the implicit Euler method, the trapezoidal rule, Ellsiepen's rule, and more. The key contribution is the application of the novel Butcher tableaus to the finite-element method and the investigation with the phase-field approach. An efficient algorithm is presented, for conclusive two-dimensional phase-field simulations proving the capability of the novel ELDIRK scheme. The higher-order convergence suggested by the new Runge-Kutta schemes is confirmed, and their effective results are demonstrated. Adaptive step size control is shown for the new low-order embedded schemes based on an empirical approach for error estimation and step size refinement.

Amplitude expansion of the phase-field crystal model for complex crystal structures

De Donno, Marcello *(Institute of Scientific Computing, Technische Universität Dresden, Germany)* 09:50

Salvalaglio, Marco *(Institute of Scientific Computing, Technische Universität Dresden, Germany; Dresden Center for Computational Materials Science (DCMS), Technische Universität Dresden, Germany)*

The phase field crystal model allows the study of materials on atomic length and diffusive time scales. It accounts for elastic and plastic deformation in crystal lattices, including several processes such as growth, dislocation dynamics, and microstructure evolution. The amplitude expansion of the phase field crystal model describes the atomic density by a small set of slowly-oscillating Fourier modes, making it possible to tackle large three-dimensional systems. However, only basic lattice symmetries have been studied so far. We present a general treatment of virtually any lattice structure using the amplitude phase field crystal model, incorporating approaches originally proposed for the phase field crystal model which enable the treatment of non-trivial lattices. We discuss the stability of selected crystal structures, focusing on non-Bravais lattices. As pivotal examples, we show that the proposed approach allows a coarse-grained description of the kagome lattice, exotic square arrangements, and the diamond lattice, hosting dislocations.

Elasticity in the phase-field crystal framework

Punke, Maik *(Technische Universität Dresden, Germany)*
Salvalaglio, Marco *(Technische Universität Dresden, Germany)*
10:10

The modeling of crystalline materials requires the resolution of microscopic details on large length and time scales to guarantee the description of lattice-dependent features as well as the dynamics of solidification.

The so-called phase-field crystal (PFC) model emerged as a prominent framework to model crystalline systems. Indeed, it describes crystalline materials through a continuous order parameter related to the atomic number density and its dynamic at relatively large (diffusive) time scales. It describes solidification and crystal growth, including capillarity, elasticity, nucleation, and motion of defects.

We discuss different ways of evaluating the mechanical stress tensor for the PFC model and compare our results to analytic solutions for a set of benchmark simulations. It is shown, that the PFC accurately predicts short- and long range behavior of the elastic field. Additionally, we apply our findings to novel aspects which were never touched before within the PFC framework, e.g. disconnections.

S06.1-04: Material modelling with metals

Date: June 2, 2023 11:00-13:00
Room: POT/112

A comparison of predictions from micropolar and strain gradient crystal plasticity theories for textured oligocrystals

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Bulut, Orhun *(Department of Aerospace Engineering, Middle East Technical University, Ankara, Turkey)*
Budnitzki, Michael *(Institute for Advanced Simulations – Materials Data Science and Informatics (IAS-9), Forschungszentrum Jülich GmbH, Jülich, Germany)*
Yalcinkaya, Tuncay *(Department of Aerospace Engineering, Middle East Technical University, Ankara, Turkey)*
Sandfeld, Stefan *(Institute for Advanced Simulations – Materials Data Science and Informatics (IAS-9), Forschungszentrum Jülich GmbH, Jülich, Germany)*

11:00

Novel additive manufacturing techniques often result in strongly textured microstructures with anisotropic grain structures. In the example of cold spraying, the grains are flattened in build direction due to severe plastic deformation. Simulations employing plasticity models based on the Cauchy continuum do not fully account for the effect of microstructure on the mechanical response. Strain gradient and micropolar crystal plasticity models possess intrinsic length scales and are sensitive to the effects of this strong texture, but are based on quite different underlying assumptions.

In this work, the performance of these nonlocal models is tested in predicting the mechanical response of such microstructures. In order to accomplish this, we calibrated the material parameters of both types of models on simple loading cases through finite element simulations and compared their performance and predictions on a set of selected oligocrystals. The advantages and disadvantages of these models for this particular application are discussed accordingly.

Investigation of propagative instabilities in aluminium alloy AW5083

Mucha, Marzena *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund Universty, Germany; Chair for Computational Engineering, Cracow University of Technology, Cracow)*
Rose, Lars *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund Universty, Germany)*
Wcisło, Balbina *(Chair for Computational Engineering, Cracow University of Technology, Cracow)*
Menzel, Andreas *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund Universty, Germany; Division of Solid Mechanics, Department of Construction Sciences, Lund University, Sweden)*
Pamin, Jerzy *(Chair for Computational Engineering, Cracow University of Technology, Cracow)*

11:20

Materials such as steel and aluminium, which are of main importance from an industrial application point of view, can exhibit so-called propagative instabilities, i.e. the Lueders bands and the Portevin Le-Chatelier (PLC) effect. They can appear simultaneously or separately along one loading path, depending on strain rate and temperature conditions. When plastic yielding occurs during tensile loading, strains can localise in a shear band, which is typically accompanied by (macroscopic) softening. The plastic front of such band can move through the sample upon further straining. When the material hardens, uniform deformation is retrieved. This phenomenon is called Lueders band formation. The PLC effect is commonly associated with Dynamic Strain Aging and related to negative strain rate sensitivity. Plastic deformation at the macroscopic level results from the initiation and motion of dislocations, whereby the motion can be stopped by solute atoms causing the dislocations to pile up. For continued loading and sufficiently large increase in stress the dislocations start to move again and the process repeats. In phenomenological description this is reflected by repetitive changes from hardening to softening in the related force-elongation diagram (serrations), while localised strain bands occur and propagate in the sample. Thereby, different PLC types can be distinguished. Type A bands propagate continuously and appear at lower temperatures and higher strain rates. Type B bands travel in a hopping manner and occur at medium temperatures and medium strain rates. Type C bands nucleate randomly and appear at higher temperatures and lower strain rates. This work is focused on the analysis of the Lueders bands and the PLC effect for aluminum alloy AW5083. Experiments on dog-bone shape specimens under tension have been performed for three strain rates. For all strain rates considered, Lueders bands are first observed, followed by (macroscopic) saturation-type hardening with PLC serrations. Moreover, different PLC types are observed. In order to computationally predict both the phenomena, a large strain thermo-visco-plastic model is proposed. Lueders bands are represented by a multi-linear hardening model, whereas the PLC effects are captured by the Estrin-McCormick model. Switch functions are also included in order to activate the respective model contributions. The model is implemented using AceGen/AceFEM for Wolfram Mathematica. A series of simulations are preformed and good agreement between experimental and numerical results is obtained. The work is supported by National Science Centre

of Poland (grant 2018/31/N/ST8/03573).

A large-strain thermoplasticity model including recovery, recrystallisation and grain-size effects

Böddecker, Merlin *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Dortmund, Germany)*
Menzel, Andreas *(Institute of Mechanics, Department of Mechanical Engineering, TU Dortmund University, Dortmund, Germany; Division of Solid Mechanics, Department of Construction Sciences, Lund University, Lund, Sweden)*

11:40

In manufacturing, thermomechanical processing steps such as hot working and annealing are commonly used to tailor the microstructure of metals to produce favourable macroscopic material properties. The underlying temperature-activated metallurgical processes of work hardening, recovery, recrystallisation and grain size evolution are driven by the stored energy of plastic deformation, i.e. dislocation density, and grain boundary energy. These processes directly affect the dislocation density, grain size and texture, resulting in a softening of the material. As recrystallisation progresses, strained grains are replaced by dislocation-free grains, which reduces the stored energy of plastic deformation and therefore the yield stress. To improve sequential manufacturing processes and predict the microstructure of the material throughout the entire process chain, physically motivated constitutive models are required that simultaneously account for the effects of recovery, recrystallisation and grain size.

In Cho et al. [1], a physically motivated recrystallisation model is proposed that unifies the effects of recovery, static and dynamic recrystallisation, grain growth and grain refinement. In the present contribution, the hypo-elasticity based model proposed in [1] is transferred to a large-strain multiplicative hyper-elastoplasticity framework. To this end, a non-associated temperature-dependent isotropic hardening law in the form of hardening-minus-recovery format is assumed, with the internal hardening variable interpreted as a measure of dislocation density. Additional internal variables of recrystallised dislocation-free volume fraction and average grain size are introduced in the hardening formulation, effectively influencing its evolution. The plasticity framework allows the evolutions of the internal variables to be modelled in terms of their true physical driving forces, namely dislocation density and grain boundary energy. In this context, static and dynamic recrystallisation effects are separated from one another by the plastic multiplier and a critical strain for the onset of recrystallisation is avoided. Finally, the Hall-Petch-type grain size effect is modelled by weighting the hardening law with a scaling factor of average grain size. For the underlying plasticity framework, an isotropic hyper-elastic Hencky-type formulation with a von Mises yield criterion is chosen. The capability of the model to predict the material response of unified recrystallisation under sequential loading is investigated by representative boundary value problems of hot working and annealing.

References

[1] H. E. Cho, Y. Hammi, A. L. Bowman, S. Karato, J. R. Baumgardner and M. F. Horstemeyer, “A unified static and dynamic recrystallization Internal State Variable (ISV) constitutive model coupled with grain size evolution for metals and mineral aggregates”, Int. J. Plast., vol. 112, pp. 123-157, 2019.

Nonlocal elasticity of Klein-Gordon type with internal length and time scales: constitutive modelling and dispersion relations

Agiasofitou, Eleni *(Karlsruhe Institute of Technology (KIT), Germany)*
Lazar, Markus *(Karlsruhe Institute of Technology (KIT), Germany)*
12:00

Generalized continuum theories like nonlocal elasticity and gradient elasticity are powerful continuum theories valid at small scales unlike classical continuum theories such as classical elasticity which cannot capture effects at small scales [1, 2]. Nonlocal elasticity considers long-range interatomic interaction, it has a close link to the underlying microstructure [1] and is valid down to the Ångström-scale [2]. Therefore, it can be considered as a generalized continuum theory of Ångström-mechanics [2].

In this work, a nonlocal elasticity theory with nonlocality in space and time is developed by considering nonlocal constitutive equations with a dynamical scalar nonlocal kernel function. The proposed theory is specified to isotropic nonlocal elasticity of Klein-Gordon type, which is an extension of nonlocal elasticity of Helmholtz type, including a characteristic internal time scale parameter in addition to the characteristic internal length scale parameter [3]. Such a nonlocal elasticity theory describes spatial and temporal nonlocal effects at small scales due to characteristic internal length and time scale parameters. The isotropic nonlocal elasticity model of Klein-Gordon type possesses only 4 constitutive parameters (2 elastic constants, 1 length scale parameter and 1 time scale parameter).

The dispersion relations for homogeneous isotropic media in the framework of nonlocal elasticity of Klein-Gordon type are analytically determined. The obtained results reveal the advantage of the proposed nonlocal elasticity model, that is, its ability to predict for the first time in the framework of nonlocal elasticity in addition to the acoustic modes (low-frequency modes), optic modes (high-frequency modes) as well as frequency band-gaps between the acoustic and optic modes. It is interesting to note that the optic modes are brought into play through the presence of a fourth-order time derivative and a characteristic time scale parameter arising from the nonlocality in time. The phase and group velocities for all four modes (acoustic and optic branches of longitudinal and transverse waves) are determined showing that all four modes exhibit normal dispersion with positive group velocity. The proposed model allows for physically realistic dispersive wave propagation [3].

References

[1] Eringen, A.C., *Nonlocal Continuum Field Theories,* Springer, New York, 2002.

[2] Lazar, M., Agiasofitou, E., Po, G., *Three-dimensional nonlocal anisotropic elasticity: a generalized continuum theory of Ångström-mechanics,* Acta Mechanica, 231, 743-781, 2020.

[3] Lazar, M., Agiasofitou, E., *Nonlocal elasticity of Klein-Gordon type: fundamentals and wave propagation,* Wave Motion, 114, 103038, 2022.

Toupin-Mindlin first strain gradient elasticity for cubic and isotropic materials at small scales

Lazar, Markus *(Karlsruhe Institute of Technology (KIT), Germany)*
Agiasofitou, Eleni *(Karlsruhe Institute of Technology (KIT), Germany)*
12:20

Nonlocal elasticity and strain gradient elasticity theories are challenging generalized continuum theories to model crystals at small scales like the Ångström-scale (see, e.g., [1,2]), where

classical elasticity is not valid and leads to unphysical singularities. The theory of first strain gradient elasticity in its modern form dates back to Toupin [3] and Mindlin [4].

A mathematical modeling of the elastic properties of cubic crystals with centrosymmetry at small scales by means of the Toupin-Mindlin anisotropic first strain gradient elasticity theory is presented [2]. In this framework, two constitutive tensors are involved, a constitutive tensor of fourth-rank of the elastic constants and a constitutive tensor of sixth-rank of the gradient-elastic constants. The 3+11 material parameters (3 elastic and 11 gradient-elastic constants), 3 characteristic lengths and 1+6 isotropy conditions are derived. The 11 gradient-elastic constants are given in terms of the 11 gradient-elastic constants in Voigt notation. The numerical values of the obtained quantities are computed for some representative cubic materials using an interatomic potential (MEAM) [2, 5]. Moreover, the isotropy conditions of strain gradient elasticity are given and discussed. A generalization of the Voigt average towards the sixth-rank constitutive tensor of the gradient-elastic constants is given to determine the 5 isotropic gradient-elastic constants [2].

References

[1] Lazar, M., Agiasofitou, E., Po, G., Three-dimensional nonlocal anisotropic elasticity: a generalized continuum theory of Ångström-mechanics, Acta Mechanica 231, 743-781 (2020).

[2] Lazar, M., Agiasofitou, E., Böhlke, T., Mathematical modeling of the elastic properties of cubic crystals at small scales based on the Toupin-Mindlin anisotropic first strain gradient elasticity, Continuum Mechanics and Thermodynamics 34, 107-136 (2022).

[3] Toupin, R.A., Elastic materials with couple-stresses, Archive for Rational Mechanics and Analysis 11, 385-414 (1962).

[4] Mindlin, R.D., Micro-structure in linear elasticity, Archive for Rational Mechanics and Analysis 16, 51-78 (1964).

[5] Po, G., Admal, N.C., Lazar, M., The Green tensor of Mindlin's anisotropic first strain gradient elasticity, Materials Theory 3 (3), (2019).

Evaluation of deformation in interactive fibre rubber composites using Woodworth-Kaliske Shape Memory Alloy material model

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Wang, Zhenbi *(Institute of Lightweight Engineering and Polymer Technology, TU Dresden)*

Woodworth, Lucas *(Institute of Structural Analysis, TU Dresden)*

Gereke, Thomas *(Institute of Textile Machinery and High-Performance Material Technology, TU Dresden)*

Kaliske, Michael *(Institute of Structural Analysis, TU Dresden)*

Modler, Niels *(Institute of Lightweight Engineering and Polymer Technology, TU Dresden)*

Cherif, Chokri *(Institute of Textile Machinery and High-Performance Material Technology, TU Dresden)*

12:40

The growing demand for intelligent systems with improved human-machine interactions has created an opportunity to develop adaptive bending structures. Interactive Fibre Rubber

Composites (IFRC) can be adapted to a desired application using the fibre reinforced rubber based actuators and the need to model and analyse these structures to achieve their maximum potential is of utmost importance. There are very few commercially developed finite element models that can predict the behaviour of Shape Memory Alloys (SMAs). The developed Woodworth-Kaliske model is a phenomenological constitutive model which is implemented in ANSYS as a user-defined function and can describe the behaviour of SMAs under mechanical loading with a possibility to apply pre-stretch to the SMA wires. The functionality of the IFRC depends on the shape memory effect of the SMA wires and on the profile shapes of the integrated SMAs. This paper discusses the importance, functionality, applicability, and limitations of the Woodworth-Kaliske SMA model on the SMA wire driven IFRC structures, by utilizing the possibility of modelling and solving for different SMA profiles and their effects on the deformations.

S06.1-05: Material modelling with metals

Date: June 2, 2023 16:00-18:00
Room: POT/112

A continuum model for disconnection-mediated interface migration: Application to the interface faceting-defaceting behavior

Qiu, Caihao *(City University of Hong Kong, Hong Kong S.A.R. (China))* 16:00
Salvalaglio, Marco *(Institute of Scientific Computing, TU Dresden, 01062 Dresden, Germany; Dresden Center for Computational Materials Science, TU Dresden, 01062 Dresden, Germany)*
Srolovitz, David *(Department of Mechanical Engineering, The University of Hong Kong, Pokfulam Road, Hong Kong SAR, China; International Digital Economy Academy (IDEA), Shenzhen, China)*
Han, Jian *(City University of Hong Kong, Hong Kong S.A.R. (China))*

Most crystalline materials of technological interest contain interfaces, which delimit the regions with distinct crystallographic orientations or crystal structures. The evolution of microstructure in materials can be described by the motion of interfaces. Hence, the equation of motion (EOM) of interfaces is theoretically important for understanding, predicting and controlling microstructure evolution. In classical approaches, interface motion by mean curvature flow is considered, for which only the reduction of total interface free energy is accounted for. However, several experiments show that the interpretations in terms of mean curvature flow do not work well for the interfaces in metals. For instance, internal stress is usually generated along with the interface motion, and externally applied stress can drive interface motion. Combined capillarity and stress effects on interface motion can be reconciled by accounting for gliding of disconnections - line defects with both step and Burgers vector character. We present an EOM which incorporates these defects for an interface of arbitrary shape in a 2D space. This EOM respects the underlying (bi-)crystallography and enables the simulation of the interface-migration-induced stress/grain rotation and the capillarity-/stress-driven interface migration.

An interesting application of the developed interface EOM is the study of the thermodynamics/kinetics associated with interface faceting/defaceting. We investigated three configurations: embedded circular grain, grain-boundary (GB) half-loop, and nominally flat interface pinned at two terminations. The main findings are as follows. (i) Inclusion of the elastic interaction associated with the dislocation character of disconnections modifies the interface morphology. In particular, it enhances faceting during microstructure evolution and enables to obtain the interface morphology of GB half-loop observed in experiments. (ii) The EOM can be used to simulate the interface motion under external stress, and the stress profoundly changes the transient interface morphology. The outcome varies with the disconnection types thus it is sensitive to underlying crystallographic aspects. (iii) The elastic interaction leads to the thermodynamic, first-order faceting-defaceting transition of a nominally flat interface, a piece of evidence widely observed in experiments but so far not explained by theoretical models.

Numerical modeling of multi-point blanking process of electrical steel

Bohdal, Łukasz *(Koszalin University of Technology, Poland)*
Kukiełka, Leon *(Koszalin University of Technology, Poland)*
Patyk, Radosław *(Koszalin University of Technology, Poland)*
Kośka, Katarzyna *(Koszalin University of Technology, Poland)*
Miksza, Mateusz *(Koszalin University of Technology, Poland)*

16:20

A new method of forming using multi-point blanking which can reduce cutting forces was discussed. In the processes of punching and blanking magnetic materials, an important problem is excessive and irregular wear of the cutting edges of the punches. The contribution proposes multi-point initiated blanking using specially designed punches, which aims to significantly reduce the punching forces needed to separate the material and punch wear. The FEM method was used to analyze the physical phenomena occurring during the process. The updated Lagrange description was used to describe the phenomena at a typical incremental step. The states of strain and strain rate are described by non-linear relationships without linearization. The description of the nonlinearity of the material was made with an incremental model taking into account the influence of the history of strain and the strain rate. The conditi on of the material after the previous treatments was also taken into account by introducing the initial states: displacements, stresses, strains and their velocities. Analyzes of the impact of the geometry of blanking tools on the values of stresses, deformations and blanking forces were carried out. Fatigue analyzes were carried out for the proposed tools. The research results may be useful for the process optimization, design of modern blanking tools used in the processing of electrical materials.

Generalizing Kocks's Natural Basis to Higher-Order Tensors

Krause, Maximilian *(Karlsruhe Institute of Technology (KIT), Germany)*
Böhlke, Thomas *(Karlsruhe Institute of Technology (KIT), Germany)*

16:40

In this work, Kocks's Natural Basis for symmetric second-order tensors [1] will be re-derived and generalized to harmonic tensor bases of arbitrary order. This formalization clarifies the fundamental relationship between the trace-deviator split of second-order tensors and the representation theory of SO(3).

In the context of anisotropic elastoplasticity, the second-order harmonic basis is shown to be more computationally efficient than corresponding Voigt or Mandel notations for isotropic, cubic and transversally isotropic materials. In the context of crystallographic texture modelling of heterogeneous materials, the higher-order extension of the harmonic basis allows easy calculation of irreducible texture tensors [2], also known as orientation tensors of third kind in fibre modelling [3].

[1] Kocks, U. F., Canova, G. R., & Jonas, J. J. (1983). Yield vectors in fcc crystals. Acta Metallurgica, 31(8), 1243-1252.

[2] Lobos Fernández, M., & Böhlke, T. (2019). Representation of Hashin-Shtrikman bounds in terms of texture coefficients for arbitrarily anisotropic polycrystalline materials. Journal of Elasticity, 134(1), 1-38.

[3] Bauer, J. K., & Böhlke, T. (2022). Variety of fiber orientation tensors. Mathematics and Mechanics of Solids, 27(7), 1185-1211.

S06.2: Material modelling with non-metals

Organizer(s): **Lion, Alexander** *(UBW München)*
Landgraf, Ralf *(TU Chemnitz)*

S06.2-01: Material modelling with non-metals

Date: May 30, 2023 13:30-16:10
Room: POT/151

Hydrothermal influences on PA 6 - dynamic mechanical analysis and viscoelastic material modeling

Kehrer, Loredana *(Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT), Germany)* 13:30
Keursten, Johannes *(Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT), Germany)*
Hirschberg, Valerian *(Institute for Chemical Technology and Polymer Chemistry, Karlsruhe Institute of Technology (KIT), Germany)*
Böhlke, Thomas *(Institute of Engineering Mechanics, Chair for Continuum Mechanics, Karlsruhe Institute of Technology (KIT), Germany)*

In the lightweight sector, polymer-based composites are increasingly applied as resource-efficient semi-structural materials [1]. In this context, polyamides are used in many different technical applications as matrix material for fiber-reinforced composites. When exposed to environmental conditions, such as temperature or humidity, the mechanical behavior and, thus, the technical performance of polyamide 6 (PA 6) is significantly affected [2]. To investigate the temperature- and humidity-dependent behavior of PA 6, dynamic mechanical analysis tests with and without humidity control were performed for samples at different humidity levels, i.e. dry-as-molded and standard atmosphere ATM-23.
Experimental results show drying effects and increased diffusion activities in the relaxation tests when the equilibrium moisture content of the sample deviates from the ambient moisture content in the test chamber. Temperature-frequency tests quantify the moisture-induced shift in the glass transition temperature. The linear generalized Maxwell model (GMM) and time-temperature superposition are applied to analyze the hydrothermal effects on the linear viscoelastic material properties. The onset of mechanical nonlinearity is discussed [3]. Based on these studies and findings, insight into the influence of moisture on material properties and the limitations of linear thermoviscoelastic modeling is obtained.

References

[1] J. Gorthofer, N. Meyer, T. D. Pallicity, L. Schottl, A. Trauth, M. Schemmann, M. Hohberg, P. Pinter, P. Elsner, F. Henning, A. Hrymak, T. Seelig, K. Weidenmann, L. Karger, and T. Bohlke: Virtual process chain of sheet molding compound: Development, validation and perspectives. Composites Part B: Engineering, 169, 133-147 (2019).
[2] L. Kehrer, J. Keursten, V. Hirschberg, T. Bohlke: Dynamic mechanical analysis of PA 6 under hydrothermal influences and viscoelastic material modeling. Journal of Thermoplastic Composite Materials, 1-35 (2023).
[3] T. Zink, L. Kehrer, V. Hirschberg, M. Wilhelm, T. Bohlke, Nonlinear Schapery viscoelastic

material model for thermoplastic polymers. Journal of Applied Polymer Science, 139(17), 1-7 (2021).

Thermoviscoelastic Modeling and Simulation of Polyamide 6

Keursten, Johannes *(Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany)*
Böhlke, Thomas *(Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany)*
14:10

In industrial applications, there is a significant demand for lightweight materials. In this context, fiber reinforced thermoplastics (FRT) are often used. From mechanical perspective, FRT exhibit thermoviscoelastic behavior [1]. As this behavior is mainly driven by the thermoplastic matrix, the behavior of the neat matrix material is of particular interest. In this work, the semi-crystalline thermoplastic polyamide 6 (PA6) is considered. An important characteristic of the thermomechanical behavior of PA6 is the glass transition. It is a thermoviscoelastic and process-dependent phenomenon which is affiliated to significant changes of the thermomechanical properties [2]. Material models of PA6 need to account for the glass transition as PA6 is applied in the vicinity of the glass transition. Based on the experimental findings documented in [3], a generalized Maxwell model (GMM) is used. Temperature-dependence is described by extended time-temperature superposition including horizontal and vertical shifts. In this work, the model is extended to include thermal expansion and calometric behavior. Based on simulations of thermomechanical load cases, implications of the model with focus on the glass transition will be discussed.

References

[1] L. Kehrer, D. Wicht, J. Wood, T. Böhlke: Dynamic mechanical analysis of pure and fiber-reinforced thermoset- and thermoplastic-based polymers and free volume-based viscoelastic modeling. GAMM Mitteilungen 41(1), 1-16 (2018)

[2] A. Lion, C. Mittermeier, M. Johlitz: Heat capacities and volumetric changes in the glass transition range: a constitutive approach based on the standard linear solid. Continuum Mechanics and Thermodynamics 29, 1061-1079 (2017).

[3] L. Kehrer, J. Keursten, V. Hirschberg, T. Böhlke: Dynamic mechanical analysis of PA 6 under hydrothermal influences and viscoelastic material modeling. Journal of Thermoplastic Composite Materials (2023).

Parameter identification for additively manufactured polymers with orthotropic material properties

Steinweller, Christina *(Clausthal University of Technology, Germany)*
Tröger, Jendrik-Alexander *(Clausthal University of Technology, Germany)*
Hartmann, Stefan *(Clausthal University of Technology, Germany)*
14:30

In recent years additive manufacturing processes, mostly known from rapid prototyping, are becoming more and more established in the production of components for end use. Whether for polymers, metals or other materials, the purpose of expanding the range of possible applications of additively manufactured components requires to perform reliable simulations. Therefore, the knowledge of a material model and the related material parameters is crucial.

A widely used additive manufacturing process for polymers is Fused Filament Fabrication (FFF). Due to the layer-wise structure of components fabricated with FFF the mechanical behavior is often considered to be orthotropic. Since the orthotropic mechanical behavior is

transferred from fiber-reinforced composites, differences between the parameter identification for orthotropic composite materials and FFF-manufactured parts are elaborated. These differences result from the possibility of FFF to manufacture specimens in almost every orientation, which allows to identify the parameters from tensile tests. In contrast, for composite materials, compression tests are necessary to determine a full set of orthotropic material parameters.

The material parameters of the underlying material model of orthotropy are identified utilizing the experimental data of various tests, including uniaxial tensile tests and three-rail shear tests, which were performed on PLA specimens printed in different orientations. The specimens were fabricated unidirectionally in order to investigate the preferred directions individually. Moreover, the use of a digital image correlation system allowed to measure homogeneous as well as inhomogeneous displacement fields during the experiments. Regarding the identification scheme, a comparison between the results of an analytical approach and a nonlinear least-squares method with finite elements is drawn, while taking into account investigations on local identifiability and the specific structure of the FFF-produced components.

Influence of process parameters on geometric and elasto-visco-plastic material properties in vat photopolymerization

Valizadeh, Iman *(Technical University of Darmstadt, Germany)* 14:50
Weeger, Oliver *(Technical University of Darmstadt, Germany)*

Photopolymerization-based additive manufacturing methods are promising approaches for fabricating intricate structures, especially on small scales, but generally limited to the use of a single material. Grayscale masked stereolithography (gMSLA) overcomes this limitation and facilitates the fabrication of structures with functionally graded material behavior. Generally, the mechanical properties and physical dimensions of the resulting parts depend on the crosslink density or degree of cure of the solidified photopolymer, which is related to the incident light energy during UV curing. In this research, we systematically investigate the influence of the main user-controllable process parameters in gMSLA, i.e., grayscale, exposure time, and layer thickness, on the resulting mechanical and geometrical properties. Based on the experimental studies, we unify these process parameters into a single controllable design parameter, the exposure intensity. We then develop elasto-visco-plastic constitutive models and geometric correction terms that describe the mechanical behavior and geometric deviations in terms of the exposure intensity. In this way, engineering design of parts with controllable and graded mechanical behaviors and reliable geometric dimensions with gMSLA is facilitated through an optimized choice of process parameters. In particular, we show that by choosing an appropriate parameter set, the print time can be significantly reduced while maintaining identical mechanical behavior. Furthermore, we show that the elasto-visco-plastic constitutive model accurately approximates the material behavior in uniaxial tension tests to failure, relaxation tests, and cyclic loadings. Overall, we observe an excellent agreement of the experimental results with numerical models for elasto-visco-plasticity during the entire process of constructing this framework for characterizing the influence of process parameters

on gMSLA. This suggests that the results should be transferable to similar material systems and 3D printing technologies.

Experimental investigations of uniaxial and biaxial cold stretching within PC-films and bars using optical measurements

Hamdoun, Ayoub *(Paderborn university, Germany)* 15:10
Mahnken, Rolf *(Paderborn university, Germany)*

Polycarbonate (PC) is an amorphous polymer which is an extremely robust material with a high tenacity, and thus suitable for a lightweight with glass-like transparency. Due to these advantageous properties, PC is often used in industry for example in medical devices, automotive headlamps, sporting equipment, electronics and a variety of other products. The PC is often subjected to uniaxial and biaxial loading conditions. Therefore, reliable material models have to take into account the various resulting experimental effects. This work deals with an extension of own developments, published before in [1], on induced anisotropy for tensile bars and films made of PC. Our objectives are to investigate uniaxial film and bar specimen and biaxial thick walled specimen with 3D-optical measurements. Here we develop different methods to determine the local inhomogeneous strain fields for different global strain rates. For the pure tension case and under the assumption of a uniaxial plane stress we use the strains to calculate the local true stress at different points of the specimen. In addition to that we investigate the effect of variations of global strain rates on the induced anisotropy. A further objective is to study the variation of the lateral displacement on the axial deformation within biaxial specimen, where we use different load cases.

References

[1] C. Dammann, I. Caylak and R. Mahnken : Experimental Investigation of PC-Films Using Optical Measurements, International Polymer Processing, 29(2), 260-271 (2014).

A Material Model for Thick, Rate-Dependent Adhesives with Delocalized Softening

Schumacher, Aaron *(Universität Kassel, Germany)* 15:30
Matzenmiller, Anton *(Universität Kassel, Germany)*

This contribution is dedicated to the development and implementation of a material model to describe the deformation behaviour of assembly adhesives. These assembly adhesives usually have a thickness of several millimeters to centimeters and can withstand high relative displacements due to their low shear modulus but highly elastic deformation behaviour above their glass transition temperature. As a basis, the isothermal and isotropic hyperelasticity theory is used to describe the highly elastic deformation behaviour up to the postcritical range by using an isochoric-volumetric decomposition of the deformation gradient. The Arruda-Boyce and Ogden models are employed here for the isochoric-elastic and volumetric-elastic description. The modelling of the rate-dependence concerning shear and bulk viscosity succeeds by extending the hyperelasticity theory to finite viscoelasticity with the generalized Maxwell model in each case. In order to model the postcritical deformation behaviour, an isotropic damage model is developed based on the energy limiting method and used to define an isochoric and a volumetric damage variable, so that the mapping of damage due to

change of shape, as well as cavitation, succeeds. Furthermore, the damage variables are delocalized to prevent pathological mesh dependence using the integral regularization method. Finally, the material parameters are determined and validated by means of measurement data due to tests at the assembly adhesive Betaforce 2850L. The results demonstrate a high prediction quality.

On Different Classes of Constitutive Descriptions in Finite Electro-Mechanics: Computational Modelling of Isotropic and Anisotropic Electro-Active Materials

Kanan, Anas *(Institute for Structural Analysis, Technische Universität Dresden, 01062 Dresden, Germany)*
Kaliske, Michael *(Institute for Structural Analysis, Technische Universität Dresden, 01062 Dresden, Germany)*

15:50

The capability of electro-active polymers (EAP) to deform largely and quasi-instantaneously under the influence of an electric field constitutes one of their main properties, which make EAP considered as favourable smart materials. The properties of a soft active material can be modified through introducing fibre or filler reinforcement into its isotropic matrix, which leads to anisotropic mechanical, electrical and electro-mechanical response of the material. Different constitutive formulations can be employed to simulate the underlying coupled behaviour. Although those distinct mathematical descriptions vary with respect to the form in which the electric field is coupled to the deformation, they are all capable of emulating the finite coupled response of EAP in an efficient manner. However, the validity of the chosen model depends on the underlying nature and coupling mechanism of the electro-active material considered. The underlying coupling mechanism of various largely deformable materials can be identified through experimental characterization. This contribution addresses the constitutive and finite element modelling of the actuation response of both isotropic and anisotropic EAP, where different material formulations are considered and implemented within a finite element framework. Those various material formulations are mathematically treated, analysed referring to the physical meaning of the predicted response and assessed based on the type of the active material considered. To this end, existing coupled electro-mechanical experiments for different classes of active materials are referred to, where it is sought to employ different constitutive models to fit the experimental observations. Within the undertaken study, the capability of the various models to realistically predict electro-mechanical instabilities, based on the type of material considered, is evaluated. Furthermore, the flexibility of those constitutive formulations to emulate various physical phenomena is assessed. Based on this study, a statement about the conditional validity and usability of those distinct models is made. Regarding the numerical implementation of the models, it is referred to an electro-mechanical Q1P0 finite element formulation. After performing the study and fitting experimental results on the material level, the actuation response of several anisotropic EAP-based structures is emulated.

S06.2-02: Material modelling with non-metals

Date: May 31, 2023 08:30-09:30
Room: POT/151

A method for characterizing hyperelastic material parameters based on the incompressible invariant plane

Buchen, Stefan *(University Siegen, Germany)* 08:30
Kröger, Nils Hendrik *(material prediction GmbH)*
Weinberg, Kerstin *(University Siegen, Germany)*

In order to characterize hyperelastic materials, tensile tests at different deformation modes are essential to determine generally valid material parameters. This circumstance is linked to the general incompressible hyperelastic material models, based on the first and second invariants of left Cauchy-Green tensor. These invariants describe the elongation and surface change and define the incompressible plane of invariants, which provides a powerful graphical relationship between deformation modes and their influence on the strain energy density. By comparing different types of deformation under the condition of equal strain energy, an equivalent deformation state can be determined. With this deformation equivalence, a method for converting stress strain relations of different deformation modes is presented and validated on experimental data. Finally, the implications of these new findings for hyperelastic material parameter characterization will be discussed.

Modelling the viscoelastic properties of elastomer blends by a diffuse interphase approach

Juhre, Daniel *(Otto von Guericke University Magdeburg, Germany)* 08:50
Voges, Jannik *(Otto von Guericke University Magdeburg, Germany)*

Elastomer blends are of high interest for tailoring materials with specific mechanical behaviour. However, while for the pure components the experimental characterization of the temperature dependent viscoelastic properties is usually well feasible, doing this for the blends is often difficult or impossible. One reason is that the blend components often have different glass transition temperatures which makes the resulting behaviour quite complex. In most cases when blending elastomers, heterogeneous morphologies are formed consisting of different regions with (nearly) pure components and finite interphases in between. Additional to the pure phases, especially these interphases influence the resulting viscoelastic properties significantly. For such cases, material modelling and numerical simulations can help to better understand the interactions between phases and interphases and to forecast the resulting viscoelastic properties. In this contribution we model and simulate an RVE of a binary blend consisting of natural rubber (NR) and styrene butadiene rubber (SBR). The modelling and the simulations are performed in the small strain regime, using linear viscoelasticity. A phase field variable is used to describe the blend morphology within the simulation. The blend morphology is based on microscopic images and the dependency on the field variable is derived from an energy formulation allowing sharp and diffuse interphases between the NR and SBR

phases. Both, sharp and different diffuse interphases are numerically investigated and their influences on the mechanical behaviour are compared to elaborate experiments.

A constitutive modelling approach to simulate time-dependent phenomena in rubber-like materials

Landgraf, Ralf *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)* 09:10
Ihlemann, Jörn *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*

Rubber-like materials exhibit complex mechanical behaviour including nonlinear stress-strain behaviour up to large strains, hysteresis, Mullins effect, permanent set, as well as time dependence. Although industrial rubbers show significant relaxation, their rate dependency is only weakly pronounced over a wide frequency range [1, 2], which is in contrast to typical viscoelastic materials like thermoplastics. Moreover, the characteristic time of relaxation depends on the rate of the previous loading sequences. In [2], these phenomena were attributed to a so-called time-rescaling behaviour of the material.

The Model of Rubber Phenomenology (MORPH) [1] offers one possibility to simulate the time-independent rubber-like material behaviour. In this contribution, possibilities are evaluated to include time-dependent effects as well. In addition, an idea presented in [2] is applied to simulate time-rescaling behaviour. The modelling approach is applied to an industrial rubber and to a polyurethane-based adhesive. Thereby, parameter identification results are presented and the applicability of the modelling approach to simulate time-dependent phenomena is evaluated.

[1] D. Besdo and J. Ihlemann (2003). A phenomenological constitutive model for rubberlike materials and its numerical applications. Int. J. Plast. 19(7):1019-1036.
[2] H. Donner, L. Kanzenbach, J. Ihlemann, and C. Naumann (2017). Efficiency of rubber material modelling and characterisation. In Constitutive Models for Rubber X (pp. 19-29). CRC Press.

S06.2-03: Material modelling with non-metals

Date: May 31, 2023 14:00-16:00
Room: POT/151

Constitutive modeling based on physics-augmented neural networks for compressible hyperelastic materials

Linden, Lennart *(Institute of Solid Mechanics, Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany)*
Kalina, Karl *(Institute of Solid Mechanics, Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany)*
Brummund, Jörg *(Institute of Solid Mechanics, Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany)*
Klein, Dominik *(Cyber-Physical Simulation Group & Graduate School of Computational Engineering, Department of Mechanical Engineering & Centre for Computational Engineering, TU Darmstadt, Germany)*
Weeger, Oliver *(Cyber-Physical Simulation Group & Graduate School of Computational Engineering, Department of Mechanical Engineering & Centre for Computational Engineering, TU Darmstadt, Germany)*
Kästner, Markus *(Institute of Solid Mechanics, Chair of Computational and Experimental Solid Mechanics, TU Dresden, Germany)*

14:00

The long-standing challenge of fulfilling all physical requirements for hyperelastic constitutive models at the same time, which have been widely debated over the last few decades, could be seen as "the main open problem of the theory of material behavior"[3]. This is particularly true for neural network (NN)-based constitutive modeling of hyperelastic materials, especially for the compressible case.

Therefore, a hyperelastic constitutive model based on physics-augmented neural networks (PANNs) is presented which fulfills all common physical requirements by construction, and in particular, is applicable for compressible material behavior. The model combines the theory of hyperelasticity established over the past few decades with the latest advancements in machine learning by expressing the hyperelastic potential as an input-convex neural network (ICNN). This potential satisfies conditions such as compatibility with the balance of angular momentum, objectivity, material symmetry, polyconvexity, and thermodynamic consistency [1,2]. To ensure that the model produces physically sensible results, analytical growth terms and normalization terms are used. These terms, which have been developed for both isotropic and transversely isotropic materials, guarantee that the undeformed state is stress-free and has zero energy in an exact way [1]. The non-negativity of the hyperelastic potential is numerically verified by sampling the space of admissible deformations states.

Finally, the applicability of the model is demonstrated through various examples, such as calibrating the model on data generated with analytical potentials and by applying it to finite element (FE) simulations. Its extrapolation capability is compared to models with reduced physical background, showing excellent and physically meaningful predictions with the proposed PANN.

[1] Linden, L., Klein, D. K., Kalina, K. A., Brummund, J., Weeger, O. and Kästner, M., Neural networks meet hyperelasticity: A guide to enforcing physics, (submitted 2023).

[2] Kalina, K. A., Linden, L., Brummund, J. and Kästner, M., FEANN - An efficient data-driven multiscale approach based on physics-constrained neural networks and automated data mining, Comput. Mech. (2023).
[3] Truesdell, C. and Noll, W., The Non-Linear Field Theories of Mechanics. 3rd ed. Springer Berlin Heidelberg, 2004.

Automated Constitutive Modeling of Viscoelastic Materials using Physics-Augmented Neural Networks

Rosenkranz, Max *(TU Dresden, Germany)* 14:20
Kalina, Karl Alexander *(TU Dresden, Germany)*
Brummund, Jörg *(TU Dresden, Germany)*
Kästner, Markus *(TU Dresden, Germany)*

The formulation of constitutive models for novel materials exhibiting complex inelastic and nonlinear behavior is still a challenging and time-consuming task. To overcome this, numerous data driven approaches involving neural networks (NNs) were developed in the recent years and have shown to be promising alternatives that automate this process without requiring any additional manual modeling effort [1]. However, using standard NNs as black-box models leads to reduced extrapolation capabilities and may violate important physical principles. Therefore, incorporating physics into the network architecture is becoming increasingly popular, either by penalizing violations during training (weak form) or by enforcing physics by construction of the NN (strong form) [2]. In this contribution, we present an approach based on a physics-augmented NN architecture which is suitable for viscoelastic materials. Thereby, the dissipation rate of the resulting constitutive model is always non-negative and thus thermodynamic consistency is enforced in a strong form. This is done by using two potentials, namely the Heltmholtz free energy and a convex dissipation potential, which are connected through Biot's relation [3]. Instead of using the tensor coordinates directly, these potentials are expressed in terms of a suitable set of invariants, forcing the model to respect the material's symmetry class. Once the training process is finished and appropriate representations of the two potentials have been found, they can be used to predict the constitutive response of the considered material. To show the ability of our approach, it is trained with synthetic data generated from a smooth random walk sequence, evaluated with a conventional viscoelastic constitutive model. Afterwards, the trained model is applied to unseen validation sequences and is compared to other, less sophisticated models concerning their interpolation as well as extrapolation capabilities, revealing a high prediction quality within a physically meaningful framework.

References:

[1] Bock, F. E., Aydin, R. C., Cyron, C. J., Huber, N., Kalidindi, S. R., Klusemann, B. (2019). A review of the application of machine learning and data mining approaches in continuum materials mechanics. Frontiers in Materials, 6, 110.
[2] Linden, L., Klein, D. K., Kalina, K. A., Brummund, J., Weeger, O., Kästner, M. (2023). Neural networks meet hyperelasticity: A guide to enforcing physics. arXiv preprint `https://arxiv.org/abs/2302.02403`.

[3] Huang, S., He, Z., Reina, C. (2022). Variational Onsager Neural Networks (VONNs): A thermodynamics-based variational learning strategy for non-equilibrium PDEs. Journal of the Mechanics and Physics of Solids, 163, 104856.

Analytical tangents for arbitrary material laws derived from rheological models at large deformations

Gypstuhl, Richard *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*
Landgraf, Ralf *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*
Wulf, Hans *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*
Ihlemann, Jörn *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*

14:40

The development of suitable material laws for various material classes is an essential preliminary work for conducting realistic simulations. Within the framework of large deformations, one recognized approach is the utilization of rheological connections allowing the construction of arbitrary models. A common method to calculate the stress response of such a material model is to formulate a set of algebraic and ordinary differential equations and to solve them numerically. In this work however, only stress equilibria between different rheological elements are formulated and directly solved by a numeric algorithm without the need to derive the typical system of algebraic/differential equations. In previous works (e.g. [1]), the computation of stress equilibria was conducted by an iterative solution procedure with a numerically calculated Jacobian matrix, giving the benefit of solving arbitrary models with one algorithm. For applications in finite element simulations, the stiffness tensor (tangent) of the material model is required. So far, all derivatives were calculated by computationally costly numeric differentiation.

In this contribution, the general approach of material modeling based on rheological connections is revisited and a refined algorithm is presented. In particular, an extension for the analytical computation of tangents is introduced, which follows the same generic and recursive methodology as the base algorithm. It is demonstrated that most intermediate terms are already provided by the stress equilibrium calculations, which significantly reduces the effort. Furthermore, the performance and stability of the analytic tangents is compared to the numerically calculated tangents using specific examples.

[1] R. Kießling, R. Landgraf, R. Scherzer, J. Ihlemann, 2016. Introducing the concept of directly connected rheological elements by reviewing rheological models at large strains. International Journal of Solids and Structures 97-98, pp. 650-667.

Microscopic Mode-Coupling Theory for Macroscopic Simulations of Elastoviscoplastic Materials

Treskatis, Timm *(Department of Mathematics, TU Dortmund, Germany)* 15:00
Steinhäuser, Sebastian *(Institute for Material Physics in Space, German Aerospace Centre (DLR), Cologne, Germany)*
Turek, Stefan *(Department of Mathematics, TU Dortmund, Germany)*
Voigtmann, Thomas *(Institute for Material Physics in Space, German Aerospace Centre (DLR), Cologne, Germany; Department of Physics, Heinrich-Heine-Universität Düsseldorf, Germany)*

Based on first principles of statistical physics, mode-coupling theory (MCT) yields a microscopic description of the highly non-Newtonian rheology of dense fluids near the glass transition. Their constitutive laws capture important effects such as static and dynamic yield stresses, as well as residual stresses that depend on the deformation history of the material. Mathematically, this rheology leads to a partial integro-differential equation for a memory function, which correlates density fluctuations over time and age of the material. The macroscopic stress in the Navier-Stokes equations is linked to the microscopic correlation function through an integral constitutive equation, as known from classical phenomenological constitutive laws in viscoelasticity.

In this talk, we will present a physics-preserving and memory-efficient numerical strategy to solve the coupled MCT - Navier-Stokes problem. Particular emphasis shall be given to the handling of the vast amounts of data that have to be kept in memory due to the complicated dependence of such flows on the entire deformation history.

We will highlight some results which exhibit unique elastoviscoplastic features that arise from the interplay of microscopic and macroscopic dynamics. Even though simulations of realistic three-dimensional flows remain out of reach due to the computational complexity of the constitutive law, we anticipate new physical insights into the phenomena of yielding and unyielding of dense fluids.

A novel thermo-mechanically coupled material model for glass above the glass transition temperature

Bögershausen, Skadi *(RWTH Aachen University, Institute of Applied Mechanics, Germany)* 15:20
Holthusen, Hagen *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*
Felder, Sebastian *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*
Brepols, Tim *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*
Reese, Stefanie *(RWTH Aachen University, Institute of Applied Mechanics, Germany)*

Thin glass products have a giant field of application in several engineering branches such as e.g. electronics, medical equipment and automobiles. The non-isothermal glass molding is a novel replicative glass processing technique enabling the realization of a cost-efficient production of surface shapes with high accuracy and complexity (see [1]). However, the application of this technology to thin glass production causes still shape distortions, cracks and

surface defects of molded parts. Therefore, these glass forming processes should be simulated by means of the combination of experimental investigation and mechanical modeling of glass above the glass transition temperature at finite strains.

Previous experimental studies have shown that the Maxwell model is a reasonable approach for an appropriate prediction of the material behavior (see e.g. [2]). Based on this viscoelastic formulation (see [3]), a thermo-mechanically consistent material law is used enabling the prediction of rheological effects noticed during the experiments. More specifically, the relaxation behavior is described by a stress-dependent relaxation time and the dissipation generated is considered as well. Furthermore, isothermal uniaxial compression tests above the glass transition temperature are conducted for different strain rates and temperatures within the experimental investigation. Combining the experimental data with the simulation, a multi-curve-fitting should lead to suitable material parameters with respect to distinct temperatures by means of a nonlinear optimization.

[1] A.-T. Vu, H. Kreilkamp, O. Dambon, and F. Klocke, Optical Engineering **55**, 071207 (2016).
[2] T. Zhou, J. Yan, J. Masuda, and T. Kuriyagawa, Journal of Materials Processing Technology **209**, 4484-4489 (2009)
[3] S. Reese and S. Govindjee, International Journal of Solids and Structures **35**, 3455-3482 (1998)

Theoretical modelling of polymer interlayer of laminated glass

Halkova, Barbora *(Czech Technical University in Prague, Czech Republic)* 15:40

Laminated glass is the composite material made of solid glass plates and polymer interlayers. While glass is almost perfectly elastic material, the polymer foil is a viscoelastic material. It exhibits time dependent behavior somewhere between purely elastic and purely viscous. Therefore, more complex theoretical models are needed instead of the theory of elasticity. Fractional calculus, i.e. the theory of derivatives and integrals of non-integer order, seems to be efficient for the theoretical modelling of viscoelastic materials. This paper presents the overview of some theoretical models and moreover compares the classical viscoelasticity with the fractional one. Classical theory of viscoelasticity employs the models composed of rheological elements such as elastic springs and viscous dampers. Meanwhile, the fractional viscoelasticity introduces the springpot element together with the principles of fractional calculus. The validation of the models will be provided by fitting parameters to the data obtained by experiments on laminated glass samples.

S06.2-04: Material modelling with non-metals

Date: June 1, 2023 16:00-19:00
Room: POT/151

Identifying microstructural properties of paper

Kloppenburg, Greta *(Bergische Universität Wuppertal, Germany)* 16:00
Li, Xiangfeng *(Bergische Universität Wuppertal, Germany)*
Dinkelmann, Albrecht *(Deutsche Institute für Textil- und Faserforschung, Denkendorf, Germany)*
Finkh, Hermann *(Deutsche Institute für Textil- und Faserforschung, Denkendorf, Germany)*
Neumann, Johannes *(Bergische Universität Wuppertal, Germany)*
Simon, Jaan-Willem *(Bergische Universität Wuppertal, Germany)*

We use CT scans of paper and paperboard to gather data of fiber network properties. A comprehensive procedure from gathering raw data over postprocessing to data analysis and the identification of suitable distribution functions is presented. The found distributions are subsequently used to generate synthetic microstructural models of paperboard for FEM simulation.

A sheet of paper is manufactured by spraying a jet of fiber-water suspension onto a mesh. Gravity, compaction and thermal treatment drive the water out. Hence, paper is comprised of a random network of interconnected fibers at the microscale. It is this fiber network that strongly influences the macrostructural properties such as in- and out-of-plane elasticity and strength. Extensive research has been conducted on network modelling to investigate the microscopic phenomena governing paper product response and failure. Simple, but computationally advantageous models idealise the fibers as beam elements, which are interconnected with rigid bonds or elastic springs. Higher levels of realism can be achieved via three-dimensional models using contact and/or cohesive zone elements. Here, we use continuum elements to discretise the tubular fibers and run a simulation of the compaction process to obtain microstructures.

On the macroscale, failure during paper processing and package instability are common. This can be attributed to defects in network properties, such as fiber volume fraction and fiber orientation. The effects remain poorly understood, despite extensive research concerning paper composition. Hence, it is worthwhile to increase our knowledge of the microstructure of paper and paperboard.

We employed non-destructive imaging methods, which have proven themselves in countless applications for various materials in the past. A total of 40 paper samples were scanned in order to obtain voxel-wise information of the fiber orientation tensors and fiber volume fractions. The distributions of both characteristics were analyzed subsequently, including the determination of in-plane fiber orientation distribution functions by applying statistical tests. These distribution functions allow to draw comparisons between different samples so that variations in fiber orientation and volume fraction can be identified. The distribution function fitting using statistical tests guarantees the selection of a suitable function. In the present

case, these are the parametric t-location scale distribution function and the non-parametric kernel smoothing function. The identified functions can be directly implemented in our fiber network models, thus enhancing their representativeness.

A constitutive model for describing decoupled material behavior in thickness and in-plane directions

Boes, Birte *(Civil Engineering Mechanics, University of Wuppertal, Wuppertal, Germany)*
Simon, Jaan-Willem *(Civil Engineering Mechanics, University of Wuppertal, Wuppertal, Germany)*
Holthusen, Hagen *(Institute of Applied Mechanics, RWTH Aachen University, Aachen, Germany)*

16:20

Paper and paperboard are gaining importance in numerous technically relevant applications, in particular in the packaging industry, because they are extremely versatile, renewable materials and easily recyclable. This leads to a growing demand for simulation tools to predict the mechanical material behavior. Due to the manufacturing process and the underlying microstructure resulting thereof, the material response is highly anisotropic. It can be divided into in-plane and out-of-plane behavior where the out-of-plane orientation is defined in thickness direction. An independent material response between in-plane and out-of-plane directions can be observed. Thus, in-plane deformations lead to in-plane stresses only and similarly for the out-of-plane direction. In existing material models, this decoupling of in-plane and out-of-plane behavior is incorporated by setting the corresponding material parameters to zero which is restrictive from a continuum mechanical point of view and limits the applicability to linear problems. Consequently, the demand arises for a continuum mechanical model that incorporates the decoupling of in-plane and out-of-plane behavior in a thermodynamically consistent manner even for large deformations and inelasticity. As the stress is the derivative of the energy, it follows to set the energy formulation as a starting point of the derivation. The Helmholtz free energy can be formulated dependent on invariants of strain measures, in particular, for example, the right Cauchy-Green tensor. Thus, a formulation of the strain measure that is divided into in-plane and out-of-plane terms is performed. By introducing structural tensors that are aligned with the preferential material directions, an in-plane structural tensor will be defined. Applying it onto the right Cauchy-Green tensor leads to a modified strain measure that captures in-plane and out-of-plane strains separately. Hence, modified invariants in terms of the modified strain measure are formulated and incorporated into the Helmholtz free energy. This directly leads to a decoupled model as separate energy terms for the in-plane and out-of-plane behavior are formulated. The framework can easily be modified in terms of different material behavior as the energy formulation can be adjusted. Due to the decoupling of the strain measures, the extension of the model to inelastic behavior is straightforward. For an easy derivation and implementation, the concept of a co-rotated intermediate configuration will be used as it is uniquely defined in comparison to the classical intermediate configuration. The model's capabilities are demonstrated by structural examples of elastic and inelastic material behavior.

Mechanics of mechanoresponsive polymeric microbubbles under ultrasonication

Khiêm, Vu Ngoc *(Department of Continuum Mechanics, RWTH Aachen University, Germany)* 16:40
Itskov, Mikhail *(Department of Continuum Mechanics, RWTH Aachen University, Germany)*

Mechanoresponsive polymers are synthesized by incorporating mechanophores - molecular units that produce chemical reactions by chain scission. Thus, the molecular-scale damage can be detected which paves the way to rationalize damage and fracture in macromolecular networks. Recently, mechanophores have been incorporated into polymeric microbubbles to optimize the ultrasound-triggered drug delivery. However, notable mechanochemical reaction can only be observed in mechanoresponsive polymers after a long period of ultrasonication. In this contribution, it is demonstrated that such limitation can be overcome by modifying the polymer topology and shell dimensions. By means of a fluid-structure interaction analysis, we find, for instance, that at a given shell thickness, suitable microbubble diameter and polymer crosslink density can maximize the chain scission over the course of the sonication in mechanoresponsive polymeric microbubbles.

Morphological implications on the mechanics of porous materials

Rege, Ameya *(Deutsches Zentrum für Luft- und Raumfahrt e.V., Germany; Keele University, UK)* 17:00

The mechanical properties of open-porous cellular materials are guided by their pore-network connectivity and their pore-wall morphologies. In this contribution, both these aspects will be discussed. First, the effect of the pore-network connectivity will be addressed. Here, the scaling exponent as observed in the power scaling relations between e.g., Young's modulus and the relative density will be explored. While the open-cell foam model calculates the exponent to be 2 [1], many porous materials demonstrate an exponent between 3 and 4 [2]. The morphological implications towards this observation will be illustrated through computational modeling and finite element calculations. Moreover, many open-porous materials show a pearl-necklace-like pore-wall morphology [3]. There, the inter-particle necks play a significant role in determining the mechanical features of such materials, particularly their mode of deformation and failure [4]. This aspect will also be explored in detail.

[1] L.J. Gibson, M.F. Ashby, The mechanics of three-dimensional cellular materials, Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences, 382 (1997) 43-59.
[2] J. Groß, J. Fricke, Scaling of elastic properties in highly porous nanostructured aerogels, NanoStructured Materials, 6 (1995) 905-908.
[3] A. Rege, S. Aney, L. Ratke, Impact of pearl-necklace-like skeleton on pore sizes and mechanical properties of porous materials: A theoretical view, AIP Advances, 12 (2022) 105108.
[4] L. Ratke, A. Rege, S. Aney, The Effect of Particle Necks on the Mechanical Properties of Aerogels, Materials, 16 (2022).

Importance of geometric parameters in modelling of porous materials – A finite element study

Chandrasekaran, Rajesh *(Department of Continuum Mechanics, RWTH Aachen University, Aachen)*
Itskov, Mikhail *(Department of Continuum Mechanics, RWTH Aachen University, Aachen)*
Rege, Ameya *(Institute of Materials Research, German Aerospace Center, Cologne)*

17:20

Porous materials consist of interconnected skeletal structure around a porous space. The skeletal structure is usually formed of a solid phase and the pores are typically filled with a fluid (liquid or gas). Porous materials are characterized by two essential geometric properties: porosity and pore size distribution (PSD), which influence their bulk mechanical properties. Porosity defined in terms of the ratio between the envelop and the skeletal densities is sufficient to describe the elastic bulk properties of porous materials. Gibson and Ashby developed a power scaling law expressing the linear relation between the elastic modulus and the relative density [1]. The PSD describes the spatial variation of the pore sizes and has recently been shown to influence the mechanical properties of porous materials [2,3]. In addition to porosity and PSD, the pore characteristics, namely pore size and shape, pore-wall size and shape, also determine the geometric properties that influence the bulk response of these materials. In this study, the importance of the above mentioned geometric parameters in the modelling of the porous materials is studied using a computational framework proposed in [4]. The bulk mechanical response under large deformation of various porous structures with PSD based on different probability density functions (PDF) and different combinations of other geometric properties under uniaxial compression is investigated. Sensitivity of mechanical response to these geometric parameters is studied. Interdependent parameters which are significantly influential are identified. By controlling these parameters, the synthesis of porous materials can be guided and optimized.

[1] L. Gibson and M. Ashby, Cellular Solids: Structure and Properties, Cambridge University Press, 1999.
[2] A. Rege, S. Aney and B. Milow, Influence of pore-size distributions and pore-wall mechanics on the mechanical behavior of cellular solids like aerogels. Physical Review E, 103, pp. 043001, 2021.
[3] S. Aney and A. Rege, The effect of pore sizes on the elastic behaviour of open-porous cellular materials. Mathematics and Mechanics of Solids, pp. 10812865221124142, 2022.
[4] R. Chandrasekaran, M. Hillgärtner, K. Ganesan, B. Milow, M. Itskov and A. Rege, Computational design of biopolymer aerogels and predictive modelling of their nanostructure and mechanical behaviour. Scientific reports, 11(1), pp. 1-10, 2021.

Analytical network-averaging: gradient damage of textile composites

tang, xuefeng *(Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany)* 17:40
Poudel, Rabin *(Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany)*
Itskov, Mikhail *(Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany)*
Jabareen, Mahmood *(Faculty of Civil and Environmental Engineering, Technion -Israel Institute of Technology, Haifa, Israel)*
Khiêm, Vu Ngoc *(Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany)*

In this contribution, we present a gradient damage model for anisotropic textile reinforcements including fiber inextensibility and fiber sliding. The analytical network averaging concept is extended to capture the mesoscopic boundary condition of the representative volume element subject to shear deformation. This approach preserves the physical meaning of the mesoscopic kinematic measure while a priori guarantees that rotations and reflections determined by orthogonal tensors within the symmetry group do not affect the response function of the anisotropic constitutive law. Such a kinematic measure is of crucial importance for material modeling of damage-elastoplasticity in an anisotropic textile reinforcement and allows for analytical descriptions of inter- and intra-ply sliding of fibers. A mixed finite element formulation is then formulated for textile reinforcements taking into account fiber inextensibility. The ill-posedness induced in the computation of the continuum damage model is treated by a Tikhonov-type regularization. The predictive capability of the computational model is demonstrated by comparing it with experimental data of dry woven fabrics.

The Inelastic Response of Woven Textile Membranes – Experimental data analysis and mechanical modeling

Makhool, Lubna *(Ruhr University Bochum, Germany)* 18:00
Uhlemann, Jörg *(University Duisburg-Essen, Germany)*
Stranghöner, Natalie *(University Duisburg-Essen, Germany)*
Balzani, Daniel *(Ruhr University Bochum, Germany)*

Due to their lightweight properties and expressive architectural shapes, woven textile membranes are increasingly in demand in numerous civil engineering applications, such as enclosing wide roof- and facade spans. They are composed of a network of interlaced yarns (warp and fill) which are covered with a rubber-like coating material. The behavior of textile membrane under uniaxial and biaxial tests is highly nonlinear and anisotropic. The effect of 'crimp interchange', i.e., the interaction between the yarns, is the main reason for the fabrics' non-linearity. A tensile load applied in a particular direction straightens crimps in the corresponding direction and increases them in the transverse direction. Moreover, the crimps in warp and fill directions are different due to the manufacturing process leading to a distinct anisotropic behavior. Furthermore, an elastoplastic response is evident in the first load cycles where considerable permanent strains are observed after unloading. The unrecoverable deformation is assumed to be associated with the internal friction between the yarns, preventing the restoration of the initial crimp once the yarns are straightened. Eventually, the

variations between the loading and unloading paths diminish, and the material reaches its elastic saturated state after three to five cycles. Several works are concerned with the saturated elastic regime, that dominates the behavior under operation conditions. However, for the design of the pre-stretch scenario, the elastoplastic models are useful where the dissipative material behavior is substantial.

In the scope of this contribution, the behavior of textile membrane under non-proportional cyclic tension applied in different directions of anisotropy and in different ratios is analyzed. Based thereon, the derivation and numerical implementation of a proper mathematical model to describe the inelastic response of the textile membrane at finite strains is presented. This model accounts for the anisotropic hyperelastic response [1], reached in the saturation region. Moreover, the plastic anisotropy is modeled by implementing the yield surface and the flow rule as a function of the structure tensor [2]. Furthermore, a fitting procedure to identify the elastic and plastic parameters is presented to show the capability of the model to simulate the behavior of textile membranes under non-proportional cyclic loading.

[1] Motevalli et al. Composite structures., 223,110908 (2019).

[2] Vladimirov et al. International Journal of plasticity., https://doi.org/10.1016/j.ijplas.2009.09.008 (2008).

Failure analysis of thick-walled composite pipes under combined loading: comparative analysis of numerical models

Menshykova, Marina *(University of Aberdeen, United Kingdom)*
Wang, Tianyu *(University of Aberdeen, United Kingdom)*
Menshykov, Oleksandr *(University of Aberdeen, United Kingdom)*

18:20

In the current study we present a comprehensive failure analysis of thick-walled multi-layered filament wound pipes subjected to combined loading. The finite element model is developed to carry out the stress and failure analysis and the model is validated by the comparison with the three-dimensional elasticity solution and the results obtained using the laminated plate theory. It could be concluded that the developed finite element model and 3D elasticity solution taking the extensional shear couplings into account shall be used for failure analysis and optimal design of composite pipes under combined loading that includes bending. Meanwhile, it is worth to notice that the analysis shows the applicability of the laminated plate theory approach for composite pipes with 0 and 90 degrees winding angles only (with some additional limitations). The detailed parametric analysis (including effects of fibres orientation, stacking sequence, magnitude of loading and layer thickness on the structural performance of the pipe) is given, and it is followed by the failure analysis and optimal design recommendations based on the modified Tsai-Hill failure coefficients.

Modeling the temperature dependent deformation behavior of fiber reinforced thermoplastics for the analysis of thermoforming processes

Ziegs, Jean-Paul *(Institute of Solid Mechanics, TU Dresden, Germany)* 18:40
Weck, Daniel *(Institute of Lightweight Engineering and Polymer Technology, TU Dresden, Germany)*
Kästner, Markus *(Institute of Solid Mechanics, TU Dresden, Germany)*

Numerical optimization of the manufacturing process of lightweight structures made of fiber-reinforced plastic (FRP) is of high importance. It can reduce the time to market and can also avoid the production of costly prototypes.

During forming of a plane textile-reinforced polymer into a three-dimensional shape, three basic deformation mechanisms - shear, tension and bending - can be observed. Since the material behavior of the polymer matrix is strongly temperature dependent, a high influence of the temperature on the deformation behavior is observed.

A hybrid modeling approach is used to decouple the almost temperature insensitive tensile and strong temperature dependent bending behavior. The reinforcement part is discretized by membrane elements and will therefore have no contribution to the bending behavior. Fibers are described as an anisotropic non-linear elastic material with orientation vectors stored at the integration points. Their tension/compression and shear behavior are decoupled by the constitutive law and can be defined by means of stress-strain curves and shear response as a function of shear angles of the fibers. In contrast, the matrix is modeled using shell elements and a thermo-elastic-plastic material law.

Experimental data for the parametrization and validation of the modeling approach are the force-displacement curves under tensile loads as well as the shear force vs. shear angle curve. The characteristic behavior for in-plane tension is determined from tensile tests on strip specimens. The typically non-linear shear force vs. shear angle curves are recorded using the picture-frame test. Since the shear force of dry fabrics is mostly influenced by the contact of adjacent fibers, an additional shear resistance due to the polymer matrix can be observed for pre-impregnated composites. Gravimetric cantilever tests may be used to determine the temperature dependent bending. Numerical studies of these tests are performed to investigate the influence of each material parameter for the respectively deformation mode.

The accordingly parameterized material model for the FRP is eventually applied in the simulation of thermoforming processes for the manufacturing lightweight structures. The comparison of the numerical and experimental results of a T-shaped bowl considering the fiber orientation and material feed is used to validate the modeling approach.

Additional parameter studies show the influence of process parameters like forming temperature, friction coefficients, initial fiber orientation and binder force on the deformation behavior of the FRP and its tendency of the occurrence of defects like the formation of wrinkles.

S06.2-05: Material modelling with non-metals

Date: June 2, 2023 08:30-10:30
Room: POT/151

Into the load bearing mechanisms of cemented granular material: a mesoscale FE approach

Komodromos, Michail *(Institute of Geotechnical Engineering and Construction Management (B-5), Hamburg University of Technology, Hamburg, Germany)*
Gorji, Mahan *(Institute of Numerical Structural Analysis with Application in Ship Technology (M-10), Hamburg University of Technology, Hamburg, Germany)*
Düster, Alexander *(Institute of Numerical Structural Analysis with Application in Ship Technology (M-10), Hamburg University of Technology, Hamburg, Germany)*
Grabe, Jürgen *(Institute of Geotechnical Engineering and Construction Management (B-5), Hamburg University of Technology, Hamburg, Germany)*

08:30

The numerical investigation of cemented granular material (CGM) has been a demanding task that requires the combination of various scientific disciplines. At the mesoscale, CGM can be decomposed into the constituents of particles, cement matrix and void pores. The combination of these constituents as found in nature or civil infrastructure projects creates a highly heterogeneous structure, whose morphology defines the mechanical response of the CGM under mechanical loading. In order to investigate the underlying mechanical phenomena down to the scale of particles, focusing on the influence of the cementation degree, a mesoscale finite element (FE) investigation was carried out.

Specifically, the composite internal structure was quantified by means of X-ray CT, providing 16 bit greyscale 3D images of the scanned micro samples corresponding to different cement saturation degrees. After being corrected against image artefacts, mainly due to beam hardening, these images were segmented, leading to precise morphological description of the three phases. These trinary images were converted into adapted FE meshes and then assigned boundary conditions to be numerically tested. The results of the simulations capture a plethora of intergranular phenomena such as stress transmission via contact, relative rolling etc. Such evidence indicates that mesh-based methods, such as the FEM, is sufficient in simulating CGMs structures, since the response of the material depends on the deformation of the cement mortar.

One step beyond, statistical analyses have been performed over the load carried by each individual particle in order to quantify the aspects of the simulated system. The grading of the particles according to the corresponding carried load confirms the highly heterogeneous nature of geomaterials, indicating uneven distribution through the existing particles. In addition, this study provided insights on the impact of the cement presence on the load distribution through the granular skeleton.

Image-based analysis of granular materials using the finite cell method

Gorji, Mahan *(Hamburg University of Technology, Numerical Structural Analysis with Application in Ship Technology (M-10), Am Schwarzenberg-Campus 4 (C), 21073 Hamburg)*
Komodromos, Michail *(Hamburg University of Technology, Institute of Geotechnical Engineering and Construction Management (B-5), Harburger Schloßstraße 36, 21079 Hamburg)*
Düster, Alexander *(Hamburg University of Technology, Numerical Structural Analysis with Application in Ship Technology (M-10), Am Schwarzenberg-Campus 4 (C), 21073 Hamburg)*
Grabe, Jürgen *(Hamburg University of Technology, Institute of Geotechnical Engineering and Construction Management (B-5), Harburger Schloßstraße 36, 21079 Hamburg)*

08:50

Efficient numerical modeling and simulation of granular material like cemented sand is a complex challenge. To simulate the interaction between the grain particles and predict the heterogeneous stress distribution, particle based methods like the discrete element method (DEM) are very well suited [1]. In the context of continuum theory, the problem can be also simulated using the finite element method (FEM), but in this case a very fine mesh along the material interfaces is needed, making the computations very costly.

To overcome this problem, the finite cell method (FCM) as an alternative to FEM, will be deployed in this contribution. The FCM is an immersed boundary method, which combines high-order finite elements with the fictitious domain approach, meshing complex geometries with a simple Cartesian grid [2]. This method is very promising for homogeneous structures, where high convergence rates are achieved. For granular materials however, which are heterogeneous and derived from computer tomography (CT) scans, several challenges occur.
The first challenge is the non-smooth (staircase) geometry description given by the CT scans. Here, a smooth geometry reconstruction based on a least-squares fit is employed, which will be directly applied on the grayscale values of the voxel models, obtained from the CT scans [3]. Now, the geometry will be described by a smooth level-set function, which then increases the accuracy of the FCM.

The second challenge is related to the discontinuities at the material interfaces, which correspond to kinks in the displacements and jumps in the strains and stresses. Since the FCM uses piecewise smooth polynomials, it is not possible to capture the discontinuous part of the solution accurately and therefore, the convergence rate deteriorates. Thus, to overcome this issue, the FCM is extended by the local enrichment, following [4]. Utilizing this extension, the FCM helps to simulate heterogeneous materials very precisely. Finally, the proposed approach will be applied to granular material like cemented sands.

References

1. De Bono, J. P. and McDowell, G. R. and Wanatowski, D. DEM of triaxial tests on crushable cemented sand. Granular Matter. Granular Matter (2014), 16:563-572
2. Düster, A. and Parvizian, J. and Yang, Z. and Rank, E. The finite cell method for three-dimensional problems of solid mechanics. Comput. Method. Appl. M. (2008) 197:3768-3782.
3. Schillinger, D. and Ruthala, P.K. and Nguyen, L.H. Lagrange extraction and projection for NURBS basis functions: A direct link between isogeometric and standard nodal finite element

formulations. Int. J. Numer. Meth. Engng (2016) 108:515-534
4. Joulaian, M. and Düster, A. Local enrichment of the finite cell method for problems with material interfaces. Comput. Mech. (2013) 52:741-762.

Modelling Rate-Dependent Inelasticity in Composites with the Scaled Boundary Finite Element Method

Eisenträger, Johanna *(Otto von Guericke University Magdeburg, Germany)* 09:10
Zhang, Junqi *(Beijing University of Technology Beijing, PR China)*
Eisenträger, Sascha *(Technical University of Darmstadt, Germany)*
Song, Chongmin *(University of New South Wales Sydney, Australia)*

Composite materials consisting of a matrix with inclusions of arbitrary shapes and distribution are nowadays used in various engineering fields. The contribution at hand aims at simulating large-scale problems, which is a challenging problem because the microstructure exerts a crucial influence on the macroscopic behaviour of structures. For this purpose, the scaled boundary finite element method (SBFEM) is chosen since it is straightforward to be combined with a quadtree-based meshing procedure because of its flexibility regarding element shapes. A major benefit of this approach is an automatic and fast discretization of microstructural images. Various matrix materials exhibit creep deformation, which is why a non-linear constitutive model for rate-dependent inelasticity is implemented into the SBFEM. Thereby, the stress update algorithm is restricted to the scaling centre of the polytope elements which results in a higher numerical efficiency and simplifies the formulation. In order to illustrate the applicability of the proposed algorithm, a metal-matrix composite under creep load is analysed. The developed constitutive model for creep is used for the matrix, whereas an isotropic elasticity model is employed for the inclusions. A microstructural image is discretized with the quadtree algorithm such that the final analysis provides detailed stress and strain fields.

Multiphasic model of early stage hydration in concrete using the Theory of Porous Media

Prskalo, Silvio *(Technische Universität Graz, Austria)* 09:30
Gfrerer, Michael Helmut *(Technische Universität Graz, Austria)*
Schanz, Martin *(Technische Universität Graz, Austria)*

Predicting the behavior of concrete is of great practical importance and as such, it has been researched throughout the years. During the initial stage of concrete maturing complex physicochemical phenomena cause considerable non-uniform deformations. Most models consider only thermo-mechanical phenomena assuming the hygral phenomena of less importance due to high liquid saturation. In order to grasp all the mentioned effects the proposed model is based on Gawin's paper [1]. The fresh concrete, modeled as porous material, is described within the well-founded framework of the Theory of Porous Media. This multiphase medium consists of a solid phase, which represents e.g. cement, gravel, etc., and a fluid and a gas phase representing their pores filled with water and dry air. Compared to the model introduced in [1], here, beside the effect of hydration-dehydration, the effect of the evaporation-condensation will be taken into account. The proposed model investigates and proves the linear connection between porosity and hydration degree for different types of

concrete, which was assumed in the model according to [1]. The presented model is implemented in the research code PANDAS. PANDAS is a multi-field finite-element solver using the variational method for solving the system of strongly coupled differential equations. Some numerical examples will be presented and those will be validated with experimental tests.

[1] Gawin, D., Pesavento, F., Schrefler, B., Hygro-thermo-chemo-mechanical modelling of concrete at early ages and beyond. Part I: Hydration and hygro-thermal phenomena. *International Journal for numerical methods in engineering*, Wiley, 2006.

Considering Orthotropic Material Behavior in a Gradient-Enhanced Damage-Plasticity Model for 3D Printed Concrete

Mader, Thomas *(University of Innsbruck, Austria)*
Schreter-Fleischhacker, Magdalena *(University of Innsbruck, Austria)*
Hofstetter, Günter *(University of Innsbruck, Austria)*

09:50

Additive manufacturing technologies such as the 3D printing of concrete are offering an increasing potential for a fast and cost-effective construction of geometrically complex structures. The mechanical behavior of 3D printed concrete (3DPC) in the hardened state is characterized by irreversible deformations, strain hardening in the pre-peak regime of the stress-strain curve and strain softening in the post-peak domain, accompanied by a degradation of the material stiffness due to damaging processes. In addition, due to the layer-upon-layer printing process of 3DPC, the mechanical behavior is significantly influenced by the interfacial bond properties between the printed filaments, resulting in an inherent orthotropic material behavior. Within the framework of finite element simulations, this orthotropic behavior is often considered as a structural effect by modeling the interfaces between the individual filaments, providing a deeper understanding of the stress distributions and damage mechanisms along the interfaces. However, such models require a high computational effort, making them unsuitable for large-scale finite element simulations of 3DPC. Thus, for providing a robust mathematical formulation of the direction-dependent material behavior of 3DPC, an extension of the well-established isotropic damage-plasticity model for concrete by Grassl & Jirasek [1] to inherent orthotropic behavior is presented. For this purpose, an orthotropic linear mapping tensor for projecting the effective stress tensor into a fictitious isotropic configuration as well as a straightforward calibration procedure of the newly introduced orthotropy parameters in the plastic regime is proposed. The model is implemented into a finite element program by means of the return mapping algorithm and it is regularized by an over-nonlocal implicit gradient-enhancement for ensuring mesh-insensitive results in the softening regime. For validation, the numerical results of material point simulations of uniaxial compression tests and 2D finite element simulations of three-point bending tests for different loading directions with respect to the principal directions of the material are compared to experimental data by Shkundalova et al. [2]. The capabilities of the constitutive model are assessed by its ability to predict the complex orthotropic mechanical behavior of 3DPC and the failure modes observed in the uniaxial compression and three-point bending tests. [1] P. Grassl, M. Jirasek, Damage-plastic model for concrete failure, International Journal of Solids and Structures 43 (22-23) (2006) 7166-7196. [2] S. Olena, Computational modelling of

material behaviour of layered 3D printed concrete, CRC Press, 2022, pages: 76-85 Publication Title: Computational Modelling of Concrete and Concrete Structures.

A micropolar Model accounting for asymmetric Behaviour of a Cold-Box Sand in Relation to Tensile and Compression Tests

Börger, Alexander *(Paderborn University, Germany)*
Mahnken, Rolf *(Paderborn University, Germany)*

10:10

The cold-box sand specimens in the work of [1] show an asymmetrical behavior in tensile and compression tests. While a horizontal surface occurs for the tensile test, a diagonal shear band develops in the specimens under pressure. This shear band is not rotationally symmetrical such that a two-dimensional model is not sufficient for its simulation. For this reason, a three-dimensional simulation becomes necessary for the geometry of a cylinder. For modelling the asymmetric behavior coupled to localization effects of the sand specimens a micropolar material model is used. This model is a special case of a micromorphic material model and has additional degrees of freedom in the form of microrotations compared to the classical continuum [2]. With micropolar continua, size effects can be mapped and the boundary value problem can be regularized when localization effects occur. As an extension of the work in [3], the flow function and the plastic potential of the micropolar model are expanded by a volumetric component analogous to [4], so that there is no local constriction and widening for tensile and compression tests, respectively. In the numerical examples for 3-D simulations the various capabilities of the model are demonstrated.

References

[1] I. Caylak, R. Mahnken, International Journal of Cast Metals Research **23**, 176-184 (2010).
[2] T. Leismann, R. Mahnken, International Journal of Non-Linear Mechanics **77,** 115-127 (2015).
[3] S. Forest, R. Sievert,Acta Mechanica **160**, 71-111 (2003).
[4] R. Mahnken, M. Schlimmer, International Journal for Numerical Methods in Engineering **63**, 1461-1477 (2005).

S06.2-06: Material modelling with non-metals

Date: June 2, 2023 16:00-18:00
Room: POT/151

Description of the deformation behavior of magnetic alginate-methylcellulose hydrogels

Czichy, Charis *(Technische Universität Dresden, Germany)* 16:00
Günther, Stefan *(Technische Universität Dresden, Germany)*
Odenbach, Stefan *(Technische Universität Dresden, Germany)*

In the field of tissue engineering regarding implants, research is being conducted on deformable scaffolds, which are colonized with stem cells. Deformation of the support structure stimulates the cells. Our own research has concentrated on magnetic hybrid materials, as these can be deformed contactless by applying an external magnetic field gradient. Since it is a novel hybrid material, the material properties such as the Young's modulus *E* as well as the deformation behavior are unknown and depend on particle concentration and time. Therefore, measurements were carried out and assumptions were made in order to formulate a model to describe the bending behavior. For this modelling a cylindrical bending beam was chosen, since it is a well-known, simple and good reproducible system. Using the theory of beams of the first order the bending curve can be described as a function of the magnetic line load, the Young's modulus, the area moment of inertia and the sample length. Hereby, the magnetic force is the simplified Kelvin force. Using an experimental setup with a Maxwell configuration for a μCT, the actual bending curves depending on particle concentration and time were detected and compared with the calculations. Taking into account the variance of the biomaterial and for a better evaluation of measured curves deviating from the theory, a range was set up instead of a single theoretical curve. Furthermore, jump tests were also carried out with this set-up and thus the time behavior of the bending could be investigated. To describe the step response, an approach was elaborated and the first parameters were determined.

Effective Diffusion Properties of Calcified Hydrogels Obtained by the Asymptotic Homogenisation

Graham, Marc *(FG Strukturmechanik und -berechnung, Institut für Mechanik, TU Berlin, Germany)* 16:20
Klinge, Sandra *(FG Strukturmechanik und -berechnung, Institut für Mechanik, TU Berlin, Germany)*

While hydrogels can be tuned to have favourable mechanical properties (e.g. strength and toughness) when dry, in most cases these qualities are lost when the hydrogel is swollen with water. To date much work has been done to coat the hydrogels or to develop hydrophobic gels and protect them from water but the recent development of calcified hydrogels by enzymatic mineralisation of calcium into the gels has achieved impressive mechanical properties [1] approaching those of biological tissues such as skin and cartilage. These relatively new materials have a heterogeneous structure and show complex diffusion behaviour. In

order to study this application-relevant property of hydrogels, the present contribution uses the homogenisation method based on a two-scale asymptotic expansion. The chosen procedure yields a homogenised diffusion tensor in terms of the volume average of its original counterpart and of solutions of auxiliary problems for unit perturbations and periodic boundary conditions. The latter are solved by using the finite element method and software library deal.II. The contribution particularly focuses on two types of microstructures. In the first case, amorphous calcium phosphate aggregates in semi-porous spheres throughout the hydrogel matrix, and in the second case the calcium forms a double inorganic-organic network. Accordingly, the representative volume elements (RVE) differ: The RVE of the first material type includes spherical, nearly-impermeable obstacles that are randomly distributed over the matrix material with a higher diffusivity. The situation is opposite concerning double-network hydrogels. Here, the matrix material is impermeable, whereas, the interconnectivity of pores is decisive for the effective diffusivity of the whole composite. The presentation compares the effective diffusivities of different materials for different size of diffusing macromolecules (proteins) as the final result. [1] Aygün, S, Klinge, S. Two-scale computational homogenization of calcified hydrogels. *Math Meth Appl Sci*. 2023; 1- 17.

A model for the evolution size and composition of olivine crystals

Haddenhorst, Hendrik Holger *(Ruhr-University Bochum, Germany)*
Hackl, Klaus *(Ruhr-University Bochum, Germany)*
Chakraborty, Sumit *(Ruhr-University Bochum, Germany)*
16:40

In this presentation, we introduce a material model to describe the evolution of olivine crystals, in particular iron-based Fayalite crystals, which are affected by the diffusion of magnesium ions. These crystals are present in magma and understanding their behavior is an important aspect in improving prediction tools for volcanic eruptions. The model describes the development of the dislocation density, the concentration of magnesium over location and time, as well as the development of the size of the crystal over time. We discuss the derivation of the model and the corresponding parameters. Furthermore, we present a numerical implementation of the model employing the platform Julia as well as a study on the influence of the various model parameters on the results.

Modelling of precipitate hardening in ferroelectric material

Bohnen, Matthias *(Technische Universität Darmstadt, Germany)*
Müller, Ralf *(Technische Universität Darmstadt, Germany)*
17:00

Precipitate hardening is well established in steel and metal processing. Recent studies have shown that this technique can also be applied on ferroelectric material, where it is an alternative to doping by foreign atoms. It effectively reduces domain wall mobility and heat dissipation, thus enhancing the mechanical quality factor of ferroelectric crystals. However, defining the optimal shape and size of the precipitates remains an open question to material scientists.
This work first aims at optimizing the geometry of precipitates inside a matrix environment

as the minimizer of both elastic and interface energy. We compare different geometry approaches with elliptical and spline interfaces. Furthermore, the model is extended by an established phase field approach to simulate domain wall formation in ferroelectric material. The effect of precipitates on domain wall movement is analyzed with finite element computations. This allows to evaluate suitable shapes and distributions of precipitates.

Second-Order Collocation Mixed FEM for Flexoelectric Solids

Tannhäuser, Kevin *(Ruhr-University Bochum, Germany)* 17:20
Kozinov, Sergey *(Ruhr-University Bochum, Germany)*

Flexoelectricity is an electromechanical coupling that exists between the electric field and the mechanical strain gradient, as well as between the mechanical strains and the electric field gradient, in all dielectric materials, including those with centrosymmetry. The governing equations used in the gradient theory to describe flexoelectricity are fourth-order partial differential equations, which require C1-continuity for straightforward numerical implementation. To this end, a new collocation-based mixed finite element method for direct flexoelectricity has been proposed, wherein a newly developed quadratic element with a high capability of capturing gradients is used. This method involves the independent definition of polynomials for the mechanical strains and electric field, which are then collocated with the mechanical strains and electric field derived from the mechanical displacements and electric potential at collocation points inside a finite element. An earlier proposed linear element, however, is unable to correctly simulate flexoelectricity due to its inability to capture all mechanical strain gradient components. To address this issue, this work employs quadratic shape functions for mechanical displacements and electric potential, requiring fewer degrees of freedom than traditional mixed finite element methods. The authors have developed a code for both the linear and quadratic elements. After verifying the linear element through numerical results from the literature, the performance of both elements has been tested on various problems. The proposed method was shown to be more accurate than existing formulations and has the potential to improve the understanding and application of flexoelectricity in dielectric materials.

Physically motivated modeling of piezoceramics in the context of mesoscale motors

Marter, Paul *(Otto-von-Guericke University Magdeburg, Germany)* 17:40
Khramova, Margarita *(York University, Toronto, Canada)*
Duvigneau, Fabian *(Otto-von-Guericke University Magdeburg, Germany)*
Orszulik, Ryan *(York University, Toronto, Canada)*
Juhre, Daniel *(Otto-von-Guericke University Magdeburg, Germany)*

The development and manufacturing of piezoelectric motors at the mesoscale (between millimeters and centimeters) is costly and challenging. One reason for this is the complex experiments for characterizing piezoceramics to predict the resulting system behavior in simulations.

To reduce the experimental effort, a common idea is to transfer the characterized material behaviour to other use cases independent of the geometry and input signals. In general, this

is challenging for phenomenological material models as these external factors have a strong influence on the determined material parameters. However, models whose parameters can be traced back to the physical behavior of the materials are particularly suitable for the transfer of material parameters to other use cases. The Jiles-Atherton (JA) model is a widely used physically motivated model for the simulation of magnetic materials. Additionally, it can be applied to ferroelectric materials and provides valuable insight into the ferroelectric behavior of piezoceramics under various conditions.

For complex applications like a piezoelectric motor, the commonly used linear model for piezoceramics is not able to adequately describe the behavior at all operation points. It is well known that the dielectric coefficients for high input voltages can not be assumed to be constant. This could also be proven by experiments for the discussed piezoelectric motor. Therefore, the JA model is used in this work to describe the nonlinear behavior of the piezoceramics. First, the polarization based on a given electric field is calculated. Then the piezoelectric matrix respectively the dielectric coefficients are determined as a function of the polarization. With the updated dielectric coefficients the resulting mechanical strains are computed considering the current electric field strength.

The model is implemented in the FE software ANSYS. The implementation is verified by previous studies from the literature. The model is then fitted to experimental data, to validate its predictions for the piezoelectric motor use case. Further work will focus on the consideration of rate dependencies in the material model.

S07: Coupled problems

Organizer(s): **Popp, Alexander** *(UBW München)*
Cyron, Christian J. *(TU Hamburg-Harburg)*

S07-01: Coupled problems

Date: May 30, 2023 13:30-16:10
Room: CHE/S89

Electro-chemo-mechanical induced fracture modeling in proton exchange membrane water electrolysis for sustainable hydrogen production

Aldakheel, Fadi *(Leibniz Universitaet Hannover, Germany)* 13:30

This work provides a framework for predicting the fracture of a catalyst-coated-membrane (CCM) due to coupled electro-chemo-mechanical degradation processes in proton exchange membrane water electrolysis (PEMWE) cells. Electrolysis in the catalyst layer (CL) bulk, diffusion of Hydrogen proton through the membrane (MEM), and mechanical compression at the interface with the porous transport layer (PTL) generate micro-cracks that influence the catalyst degradation. Based on the experimental observations, we propose a new theoretical formulation along with the constitutive framework to help understanding and providing a reliable description of the stated multi-physics problem. The computational modeling of crack formation in the CL bulk is achieved in a convenient way by continuum phase-field formulations to fracture, which are based on the regularization of sharp crack discontinuities. The model performance is demonstrated through two representative boundary value problems, representing the cell setup and working of the PEMWE cell.

A volumetric heat source model for the identification of the mushy zone in laser beam welding.

Hartwig, Philipp *(Institut für Mechanik, Universität Duisburg-Essen, Germany)*
Scheunemann, Lisa *(Lehrstuhl für Technische Mechanik, RPTU Kaiserslautern-Landau, Germany)*
Schröder, Jörg *(Institut für Mechanik, Universität Duisburg-Essen, Germany)* 14:10

Laser welding is a metal working process that, with its high advance speed and low thermal distortion, is used more frequently nowadays in industry. During welding, the solidification front is located in the so-called mushy zone, which forms the transition region between the solid material and the already melted material. Inside the mushy zone, areas of included melt can occur at the high speeds during laser beam welding, which may cause cracking due to shrinkage when the molt solidifies.

The properties in the solidification region depend on various parameters. Process parameters such as the welding speed and the resulting temperature gradient in the heat affected zone as well as internal factors such as the chemical composition can have an influence on the likelihood of solidification cracking. In order to investigate the heat affected zone more precisely, different models describing the laser beam as heat source are discussed. The aim is to develop a volumetric heat source model, which is based on the Goldak model and resembles the temperature distribution given by the Lame curves, see [1] and [2]. The Goldak

model is based on a Gaussian distribution within a double ellipsoid geometry. It assumes an elliptical structure and introduces a division into front and rear parts. For the Lame curves the geometry of the weld pool can be extracted from a previous CFD simulation calibrated with experimental results. The idea behind the use of Lame curves is based on this geometry to generate a surface of constant temperature. This structure is then used as a heat source in a FEM simulation to calculate the temperature distribution within the system.

The modified volumetric heat source model mimicks given experimental results of the weld pool geometry and thermal properties of the Lame curves and combines the variability of the Goldak model. The intrinsic and process dependent regulation of the energy input in this newly developed model enables a simplified recalibration of the model. Numerical examples of the models are discussed for different settings of the process parameters with a focus on the heat distribution and the possibility of identification of the mushy zone.

References:
[1] J. Goldak, A. Chakravarti and M. Bibby. A New Finite Element Model for Welding Heat Sources. Metal- lurgical Transactions B, 15B, 299-305, 1984.
[2] A. Artinov, V. Karkhin, N. Bakir, X. Meng, M. Bachmann, A. Gumenyuk and M. Rethmeier. Lame curve approximation for the assessment of the 3D temperature distribution in keyhole mode welding processes. Journal of Laser Applications, 32, 022042 (8 pages), 2020.

Application of DeepONet for Temperature Prediction in Powder Bed Fusion Process

Safari, Hesameddin *(Institute for Computational Modeling in Civil Engineering, TU Braunschweig, Germany)*
Wessels, Henning *(Institute for Computational Modeling in Civil Engineering, TU Braunschweig, Germany)*

14:30

Nowadays, additive manufacturing using powder bed fusion (PBF) technology has significantly improved the accuracy and efficiency of manufacturing processes in various industries. A better understanding of physical phenomena in additive manufacturing through numerical simulations facilitates us in optimizing this technique for each product. For example, in selective laser sintering (SLS) [1] laser power is used to bind powdered material into solid structures. In this process, tool path selection directly affects the stress distribution in the built product by controlling the average temperature gradient during the building process. Consistent simulation of these rapid physical phenomena using standard solvers requires very fine time steps and high spatial resolutions, which might cause a computational burden. These constraints could severely restrict the optimization and sensitivity analyses of the process in which many scenarios are to be considered. In recent years, machine learning algorithms and data-driven approaches have gained popularity in scientific computing, where fast and reasonably accurate solutions are to be addressed. Most recently, DeepONet (learning operators using deep neural networks) [2] has emerged as a powerful tool for learning non-linear and complex operators with smaller generalization errors compared to other well-known architectures. Under appropriate training, it could effectively serve as a solution operator of partial differential equations (PDEs). Here, DeepONet is employed to infer a consistent temperature field in the PBF processes. We train the network with different heat source paths as well as the heat source powers and investigate how consistent our network would be for

unseen scenarios. As a purely data-driven approach, one major drawback of DeepONet is that it requires lots of labeled data for supervised learning. In many engineering applications, such as PBF simulations, obtaining several training data from expensive numerical solvers would not be that convenient. In order to improve the accuracy and reduce the generalization errors, even without previous solutions, the combined DeepONet-PINN (physics-informed neural networks) algorithm is developed in which a physics-informed DeepONet could be trained in an unsupervised manner. Our proposed framework could also be efficiently employed to obtain an optimal tool path in the SLS process.

References

[1] Kim, D.H., Zohdi, T.I. "Tool path optimization of selective laser sintering processes using deep learning", Comput Mech 69, 383-401 (2022). https://doi.org/10.1007/s00466-021-02079-1

[2] Lu, L., Jin, P., Pang, G. et al. "Learning nonlinear operators via DeepONet based on the universal approximation theorem of operators", Nat Mach Intell 3, 218-229 (2021). https://doi.org/10.1038/s42256-021-00302-5.

Basics and challenges in IGA-based modelling of temperature and hydrodynamic properties in the context of wet grinding

Thunich, Paul *(Institute of Dynamics and Vibrations, TU Braunschweig, Germany)* 14:50
Tong, Yan *(Institute of Dynamics and Vibrations, TU Braunschweig, Germany)*
Müller, Michael *(Institute of Dynamics and Vibrations, TU Braunschweig, Germany)*
Schömig, Oliver *(Institute of Machine Tools and Production Technology, TU Braunschweig, Germany)*
Arafat, Robar *(Institute of Machine Tools and Production Technology, TU Braunschweig, Germany)*
Herrmann, Christoph *(Institute of Machine Tools and Production Technology, TU Braunschweig, Germany; Fraunhofer Institute of Surface Engineering and Thin Films (IST), Braunschweig, Germany.)*

In grinding processes, process parameters are currently set based on experience or empirical trial-and-error tests, since few knowledge about basic interactions exists and contrary influences must be balanced. Especially when developing new cutting fluids, a conflict between cooling effects and hydrodynamic load-bearing effects arises. To resolve this conflict, a model should be developed to investigate interactions and optimise wet grinding processes.

First investigations model a cylindrical roller bearing profile as a rough approximation of a grinding wheel describing the pressure built-up, cavitation and thermal effects, mainly due to viscous shearing. Numerical analysis is done via isogeometric analysis (IGA) using NURBS, so far mainly used for structural problems, as a fast way of computing parameters in hydrodynamics, especially for complex geometries.

For the description of the influence of the cutting fluid in wet grinding processes, a thermal model, first describing the heat production due to fluid shearing was developed. In this context, increasing the used dimensions for modelling the pressure built up and cavitation regimes by adding the dimension normal to the gap direction was necessary since fluid velocity distribution in that direction is usually non-linear. Due to fast rotating grinding-wheels and the high delivery pressures of the cutting fluids, fluid velocities in wet grinding are high and

the heat equation is therefore convection-dominated. In addition, the small number of nodes used in IGA (e.g., for the aforementioned question 100 nodes) leads to large element sizes, producing spurious numerical oscillations based in the Galerkin approach and stabilisation is needed. In contrast to widely used SUPG-stabilisations for linear elements, evaluation of the second derivatives and their transformation is necessary to compute the stabilised solution.

Using stabilisations for the computation of pressure and cavitation, this paper presents a SU-stabilisation for better convergence followed by a SUPG-stabilisation for more accurate solutions in the Newton-procedure, and SUPG-stabilisation for the heat equation. The IGA results are in good agreement with CFD-solutions elaborated with the commercial tool Ansys Fluent even for complex geometries like sections of a grinding wheel. In addition, the heat distribution in the surrounding solids is considered by means of domain coupling using the mortar method.

NURBS-based IGA in combination with stabilisation allows for fast computation using only a few nodes. By that, the model is a valuable basic approach and has a large potential for research on complex questions, construction of complex models and even iterative optimisations in the field of wet grinding.

Chemo-mechanical modelling of the breathing effect during lithiation and delithiation in Li-Si batteries

Dittmann, Jan *(Kiel University, Germany)*
Stern, Jan-Ole *(Kiel University, Germany)*
Beiranvand, Hamzeh *(Kiel University, Germany)*
Wulfinghoff, Stephan *(Kiel University, Germany)*

15:10

Due to their high energy density and high cell voltage, lithium-ion batteries have become the most prominent battery type used in electronic devices today. However, research still aims to reduce costs, increase sustainability and improve battery performance by new combinations of electrode and electrolyte materials. One promising candidate for a superior anode material is silicon due to its ability to form an alloy with lithium, which leads to a much higher theoretical capacity in comparison to commonly used electrodes that store lithium-ions by intercalation. However, the main disadvantage of silicon is the large volume change (breathing) during lithiation and delithiation, which results in high mechanical stresses, cracking and ultimately failure of the battery. Structuring the anode is a possible solution to minimize these stresses but requires tools to better understand and predict the material behavior.
Here, we present a chemo-mechanical FEM model for the breathing effect of the silicon anode during lithiation and delithiation. The model is based on the framework for gradient extended standard dissipative solids [1]. It couples diffusion of lithium ions, phase transformation with a moving phase boundary and the related volume changes which lead to mechanical stresses in the material. The driving force for diffusion is given by the gradient of the electrochemical potential. Phase transformation and phase boundary movement is described by a phase field with a double obstacle potential [2], which is implemented using a micromorphic approach [3] to shift the constraint of the order parameter $\xi \in [0, 1]$ from the nodes to the Gauss points. Further, the model is implemented for finite strains and discriminates between

elastic deformations and chemical volume expansion by splitting the deformation gradient multiplicatively into two respective parts.

Determination of the effective properties of solid oxide fuel cell electrodes by applying a computational homogenization approach

Langner, Eric *(TU Dresden, Institute of Solid Mechanics, Germany)*
Makradi, Ahmed *(Luxembourg Institute of Science and Technology, Luxembourg)*
El Hachemi, Mohamed *(Luxembourg Institute of Science and Technology, Luxembourg)*
Belouettar, Salim *(Luxembourg Institute of Science and Technology, Luxembourg)*
Wallmersperger, Thomas *(TU Dresden, Institute of Solid Mechanics, Germany)*

15:30

The current total energy supply is 80% fossil fuels. In order to reduce the CO_2 consumption in the world, fuel cells will be indispensable for the environmentally friendly generation of electrical energy. Solid oxide fuel cells operate at high temperatures and have high efficiency compared to other types of fuel cells. They also have a higher tolerance with respect to impurities and are therefore suitable for different fuels. However, many experimental studies show that the composition and the microstructure morphology of porous electrodes have a great influence on the durability and conversion efficiency of electrochemical devices. For instance, in order to enable the fuel and the air to flow to the cell active sites in which the electrochemical reactions take place, the microstructure must exhibit both sufficient porosity and high pore connectivity. To establish a relationship between the specific microstructure of the electrodes and the performance of the overall fuel cell, an estimate of the macroscopic material parameter is required. Due to time-consuming and cost-intensive reasons, both a large amount of experiments with various physical or geometrical properties and of numerical simulations with a fully resolved microstructure are nearly impossible. Therefore, a first-order computational homogenization method capable of capturing anisotropic and nonlinear effects is applied in the present study. Due to the multiphysics fields involved in describing the nature of the electrodes, a multi-field homogenization framework is developed and implemented in a finite element tool. This procedure is supposed to enable the material modeling of heterogeneous electrodes. The effective properties can be used to conduct numerical simulations on the fuel cell level in order to obtain correlations between the microstructure morphology and the performance.

S07-02: Coupled problems

Date: May 31, 2023 08:30-09:30
Room: CHE/S89

Coupling strategies for the cardiovascular system

Schussnig, Richard *(University of Augsburg, Germany)* 08:30
Kronbichler, Martin *(University of Augsburg, Germany)*

Robust and efficient numerical modeling of hemodynamics is a particularly challenging problem in the medical field. Simulation tools applied in the clinical context can improve management and prognosis of life-threatening diseases or allow studies on digital cohorts. Virtual surgery can be performed to identify optimal treatment variants, leading to minimal patient risk and reduced cost. Despite great progress in the field of computational (bio-)mechanics, full-scale patient-specific simulations are yet to be routinely applied for clinical support. Key problems in this regard are overwhelming simulation turnaround times, insufficient robustness and low accuracy due to overly restrictive assumptions. To overcome the most pressing limitations, we combine (i) patient-specific cardiovascular models, (ii) accelerated Robin coupling strategies and (iii) state-of-the-art matrix-free Discontinuous Galerkin solvers within the open-source software framework ExaDG [1]. A partitioned algorithm is employed to strongly couple the generalized Newtonian fluid and three-dimensional bulk continuum. Special care is taken to counteract the added-mass effect triggered by in-vivo density ratios, combining Robin coupling conditions and interface quasi-Newton methods within a semi-implicit coupling procedure as recently presented by the authors [2]. Together with filtering techniques, re-using past interface iterates further accelerates the iterative scheme and improves stability considerably. The computational framework ExaDG implements various time discretization schemes for incompressible flows, namely, higher-order splitting or projection methods and classical monolithic formulations of the incompressible Navier-Stokes equations, see, e.g., Kronbichler et al. [3]. We critically compare the various implemented fluid-structure interaction solvers adopting physiological flow conditions and physical parameters, while considering aspects specific to hemodynamics such as 3D-0D multi-scale models of the downstream vasculature and external tissue support.

[1] D. Arndt, N. Fehn, G. Kanschat, K. Kormann, M. Kronbichler, P. Munch, W. A. Wall, and J. Witte. ExaDG: High-order discontinuous Galerkin for the exa-scale. In H.-J. Bungartz, S. Reiz, B. Uekermann, P. Neumann, and W. E. Nagel, editors, Software for Exascale Computing - SPPEXA 2016-2019, 189-224, Springer International Publishing, 2020.
[2] R. Schussnig, D.R.Q. Pacheco, M. Kaltenbacher, T.-P. Fries. Semi-implicit fluid-structure interaction in biomedical applications. Computer Methods In Applied Mechanics And Engineering 400, 115489, 2022.
[3] M. Kronbichler, N. Fehn, P. Munch, M. Bergbauer, K.-R. Wichmann, C. Geitner, M. Allalen, M. Schulz, and W. A. Wall. A next-generation discontinuous Galerkin fluid dynamics solver with application to high-resolution lung airflow simulations. In Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, 1-15, 2021.

Coupling instable pore geometries with local flow to allow for high attenuation at low frequencies

Kurzeja, Patrick *(TU Dortmund, Institute of Mechanics, 44227 Dortmund, Germany)*
Quintal, Beatriz *(University of Lausanne, Institute of Earth Sciences , 1015 Lausanne, Switzerland)*

08:50

Attenuation at low frequencies is a key requirement for many industrial systems, e.g., multi-story buildings, machinery and aircraft. Interestingly, an attenuation mechanism at low frequencies is observed in natural, fluid-filled materials such as rocks, namely, in the form of local flow [3-5]. The energy loss is caused by fluid exchange between pores of different compliance [2]. The present work aims at harnessing this natural mechanism in highly elastic structures that allow for drastic pore compression [1]. Instabilities at the pore level even allow to control and to amplify the dissipative effect of local flow beyond the limit of natural materials. Silicone samples illustrate the basic requirements that make artificial pore geometries prone to local flow. Numerical simulations of a prototype structure subsequently demonstrate the impact of various geometric and material parameters. A key to maximum attenuation is the fluid-structure interaction inside the pores. The fluid viscosity and permeability between the pores determine the characteristic frequency. The stiffness ratio between the structure and the pore fluid determines how much energy can be dissipated but also whether instabilities can evolve to trigger local flow at all.

[1] Cohen, T., P. Kurzeja and K. Bertoldi, 2017. Architected squirt-flow materials for energy dissipation. Journal of the Mechanics and Physics of Solids 109, 22-33, https://doi.org/10.1016/j.jmps.2017.08.003.
[2] O'Connell, R. J., and B. Budiansky, 1977. Viscoelastic properties of fluidsaturated cracked solids. Journal of Geophysical Research 82, 5719-5735, https://doi.org/10.1029/JB082i036p05719.
[3] Pimienta, L., J. Fortin and Y. Guéguen, 2015. Bulk modulus dispersion and attenuation in sandstones. Geophysics 80, D111-D127, https://doi.org/10.1190/geo2014-0335.1.
[4] Pimienta, L., J. Fortin and Y. Guéguen, 2015. Experimental study of young's modulus dispersion and attenuation in fully saturated sandstones. Geophysics 80, L57-L72, https://doi.org/10.1190/geo2014-0532.1.
[5] Quintal, B., E. Caspari, K. Holliger, and H. Steeb, 2019. Numerically quantifying energy loss caused by squirt flow. Geophysical Prospecting 67, 2196-2212, https://doi.org/10.1111/1365-2478.12832.

Drag modeling for the flow-induced reconfiguration of a tapered flexible ribbon

Schoppmann, Karl *(TU Dresden, Germany)*
Löhrer, Bastian *(TU Dresden, Germany)*
Fröhlich, Jochen *(TU Dresden, Germany)*

09:10

Reconfiguration describes a mechanism of a flexible body that changes its geometry due to external fluid loads, leading to a reduced drag which would otherwise grow proportionally to the velocity squared, in the pressure-dominated regime. In the particular case of the highly flexible ribbon investigated experimentally in [1], reconfiguration first yields a quadratic drag

regime with increasing flow velocity, but after a critical threshold is passed, the drag force becomes independent of the flow velocity over a remarkably wide range. For this experimental reference configuration, the presenting authors published first numerical results of Large Eddy Simulations (LES) in [2], reporting static reconfiguration and a complex, three-dimensional laminar, transitional and turbulent fluid motion around the trapezoidal ribbon. In the present contribution, the distribution of fluid loads along the ribbon is investigated in a self-similar framework and a new improved model for the local drag coefficient is derived from the characteristics of the surrounding flow. A subsequent application of the proposed model shows an improved prediction of the drag reduction, quantified by the dimensionless reconfiguration number. Total drag reduction is analyzed in terms of two components which represent the relevant mechanisms responsible for reconfiguration, area reduction and streamlining. It is found that the first one dominates in the regime of large deformation compared to the latter. For a small intermediate regime between quadratic and constant drag behavior, the derived model predicts - in accordance with the results of the LES - a slightly positive Vogel exponent V, i.e. an increased drag which is proportional to the (2+V) power of the oncoming flow velocity. This counter-intuitive phenomenon of reconfiguration is finally related to the analysis of the flow around the ribbon.

[1] T. Barois and E. de Langre (2013): Flexible body with drag independent of the flow velocity. J. Fluid Mech. 735, R2.

[2] K. Schoppmann, B. Löhrer, S. Tschisgale, J. Fröhlich, E. de Langre (2021): An efficient solver for a Cosserat rod of non-constant width applied to a problem of fluid-structure interaction. PAMM 21:1 e202100152.

S07-03: Coupled problems

Date: May 31, 2023 08:30-09:30
Room: CHE/184

A diffusion-driven biofilm growth model based on an extension of the Hamilton principle

Klempt, Felix *(Leibniz Universität Hannover, Germany)* 08:30
Soleimani, Meisam *(Leibniz Universität Hannover, Germany)*
Junker, Philipp *(Leibniz Universität Hannover, Germany)*

For the last five decades, oral implants are a highly successful and long-term treatment method for tooth loss. In some cases, however, oral implants lead to peri-implantitis, an infection of the gum and bone, which itself can result in bone loss and implant failure. Peri-implantitis is caused by bacteria forming a so-called “biofilm” on the implant surface. In order to develop prevention strategies, a deep understanding of biofilms, in general, is necessary. In silico models have proven to be viable tools to perceive the mechanisms contributing to biofilm formation. Besides, they are complementary to in vitro as well as in vivo experimental observations. Current biofilm growth simulations in literature are using mainly one of two approaches. Either a volumetric approach is used in which the deformation tensor is split in a growth and a deformation part, or a density-based approach is chosen in which the local density evolves according to an evolution equation. Neither of these approaches, which are phenomenologically motivated, can ensure that the model complies with the second law of thermodynamics. The reason is that the growth phenomenon, unlike classical deformation in solids, usually happens in an open system in which entropy as well as energy is exchanged through the boundaries and it poses serious challenges to thermodynamic consistency conditions. The novel model presented in this work is derived from an extended Hamilton principle. It can not only combine the kinematic-volumetric approach with the density-based approach but also, due to its derivation through Hamilton’s principle, the laws of thermodynamics are inherently fulfilled.

The biofilm model is homogenized and solved using finite element methods. The model is capable of capturing directional growth towards a source of nutrients. One of the superiorities of the utilized method, in comparison to the purely kinematic-based approaches, is that the self-contact scenario is not an issue. In fact, the biofilm can grow around the obstacles and it is remerged into itself. The model, as stands now, consists of only one species of bacteria and a nutrient source. The mathematical formulation can be readily extended to the multispecies system. Moreover, the impact of antimicrobial agents, which serve as a negative nutrient, can be incorporated. These are left for future work.

Mathematical modeling of biological ion channels

Keller, Christine *(Weierstrass Institute for Applied Analysis and Stochastics (WIAS))* 08:50
Fuhrmann, Juergen *(Weierstrass Institute for Applied Analysis and Stochastics (WIAS))*
Landstorfer, Manuel *(Weierstrass Institute for Applied Analysis and Stochastics (WIAS))*
Wagner, Barbara *(Weierstrass Institute for Applied Analysis and Stochastics (WIAS))*

Many physiological functions are regulated by ion channels, which makes them an important target for the development of new therapies and medications. Those pore-forming transmembrane proteins are investigated in the laboratory by studying the current response as a function of an applied potential. We developed a PDE-based model-framework to support the interpretation of experimentally measured current-voltage relations. Based on non-equilibrium thermodynamics, mixing theories and electrodynamics, we describe ion activities in the channel. The model accounts for space and correlation phenomena such as space-charge competitions and excluded-volume effects. In this work, we focus on calcium ion channels as an example and have included a selectivity filter as an embedded domain within the pore. To ensure selectivity, transfer reactions are introduced as Neumann interface conditions. The resulting system of drift-diffusion equations is numerically solved using a thermodynamically consistent finite-volume method. We calculated and studied current-voltage curves for different membrane potentials, varying ion concentrations and properties of the channel protein.

On numerical aspects of forward and inverse analysis of a two-phase bone model

Blaszczyk, Mischa *(Ruhr-University Bochum, Germany)* 09:10
Hackl, Klaus *(Ruhr-University Bochum, Germany)*

In previous contributions (e.g. [1,2]), we established a multiscale, multiphase material model of cancellous bone, using the finite element square method and two phases on the microscale. An important application for our model is the usage of sonography as a future diagnosis tool for the early detection of osteoporosis. This disease makes the bone softer and more likely to fracture. While our previous results were already promising, some important aspects were not sufficiently considered, which limited the applicability of our model. In this talk, after shortly reintroducing the basic model, we present important improvements concerning two parts. First, we split the macroscopic model into different areas, which allows a finer differentiation between the bone phases and the inclusion of a surrounding medium. Second, we show, how the inverse problem - obtaining information about the bone composition from simulation data - can be solved accurately by using artificial neural networks. We show numerical results for all problems.

References:

[1] Blaszczyk, M., Hackl, K., “Multiscale modeling of cancellous bone considering full coupling of mechanical, electric and magnetic effects”, Biomech. Model. Mechanobiol, (2021)

[2] Stieve, V., Blaszczyk, M., Hackl, K., “Inverse modeling of cancellous bone using artificial neural networks”, Z Angew Math Mech, (2022)

S07-04: Coupled problems

Date: May 31, 2023 14:00-16:00
Room: CHE/S89

Fluid-structure interaction of a dynamic seal with 3D-printed surface

Graf, Matthias *(Hochschule Emden/Leer, Germany)* 14:00
Lankenau, Tobias *(Hochschule Emden/Leer, Germany)*

Additive manufacturing (AM) methods find more and more applications in the manufacturing of machine parts. One consequence of this method is that generated surface qualities are typically lower than in other processes. This becomes especially relevant when the surface quality is the critical for the mechanical function: This is the case in dynamic sealing technologies, e.g. in seals between moving rod and a hydraulic cylinder. Between the seal lip and the polished rod a thin lubrication film is established, with the goals of low coefficient of friction and minimal leakage. How good these goals are reached depends on the surface quality of the seal. For spare part production of seals AM methods are under investigation, that have a surface defined by layers from fused deposition modelling (FDM). We apply a coupled model for fluid-structure interaction of the elastic seal and the film flow. This model provides information on leakage flow, pressure distribution, forces and the coefficient of friction. Results change when the "ideal" seal lip is repaced by the seal lip geometry from FDM. The continuous loss of solid-body-contact is replaced by a stepwise loss of of contact for the FDM surface. Furthermore the coefficient of friction inceases for the FDM surface due to additional losses in the more complex fluid flow.

Fluid-structure interaction with fully coupled mesh generation

Schwentner, Teresa *(TU Graz, Austria)* 14:20
Fries, Thomas-Peter *(TU Graz, Austria)*

The modeling and simulation of fluid-structure interaction (FSI) involves the two-way coupling of a fluid flow and a deforming structure. The fluid exerts a load on the structure, the structure deforms, and, hence, the fluid flow changes which leads to an altered loading on the structure. To accomplish this coupling, the domain has to be updated after each time step, leading to a change of the fluid mesh [1]. Various mesh update methods have been presented where an initial mesh is generated and then updated after each timestep. Each method comes with different levels of complexity and its own advantages and disadvantages e.g., [2, 3]. An earlier contribution proposed the idea of a fully integrated mesh generation [4]. Herein, FSI simulations with fully integrated mesh *generation*, rather than updates, highlight the advantages of this approach, such as robustness and applicability for large deformations. Instead of updating the mesh in each time step, a new mesh for the fluid domain is generated based on the deformation of the solid domain. An advanced structured meshing algorithm based on building blocks allows this integrated mesh generation approach. An initial set of coarse-scale building blocks is generated by the user, representing the topology and rough initial position of the solid and the fluid. Further information are the exact geometry at the boundary and the deformed position of the fluid-structure interface plus grading information to obtain a high-quality fluid mesh. Transfinite maps are used to generate elements inside

the building blocks with any desired resolution and order. This also enables FSI-simulations with hp-FEM [4]. Numerical results confirm the success of this approach.

[1] Richter, T.: Fluid-Structure Interactions: Models, Analysis and Finite Elements. Springer International Publishing, Cham, 2017.
[2] Stein, K.; Tezduyar, T.; Benney, R.: Mesh moving techniques for fluid-structure interactions with large displacements. J. Appl. Mech., ASME, 70, 58-63, 2003.
[3] Jendoubi, A.; Deteix, J.; Fortin, A.: A simple mesh-update procedure for fluid-structure interaction problems. Computers & Structures, 169, 13-23, 2016.
[4] Fries, T.P.; Bošnjak, D.; Schussnig, R.: Fully integrated mesh generation in fluid-structure interaction, 8th European Congress on Computational Methods in Applied Sciences and Engineering, Oslo, Norway, 2022.

Large Eddy Simulation of the flow over a canopy with spanwise patches

Fröhlich, Jochen *(Technische Universität Dresden, Germany)*
Löhrer, Bastian *(Technische Universität Dresden, Germany)*
14:40

In the present contribution, numerical simulations of the flow over idealised aquatic canopy patches are presented. These patches consist of flexible blades interacting with the surrounding flow. The physical parameters governing the flow, the characteristics of the blades and their positioning within the vegetation patch are identical to a previously studied homogeneous scenario where the Monami phenomenon occurs. A recently developed own numerical method capable of representing such a situation is used to generate high resolution data for the turbulent flow and the motion of the individual structures. The talk will concentrate on the physical analysis of the data, highlighting processes related to the presence of the patches.

Numerical study of the motion of an aquatic canopy envelope in relation to the surrounding fluid

Löhrer, Bastian *(Technische Universität Dresden, Germany)*
Fröhlich, Jochen *(Technische Universität Dresden, Germany)*
15:00

In the present contribution, numerical simulations of the flow over aquatic canopies are presented. The canopies consist of highly flexible slender rods closely interacting with the surrounding flow. The regime addressed is the one of particularly high Cauchy numbers, around 25000, which is characteristic for very flexible structures with substantial reconfiguration. While such canopies constitute a central element in river hydraulics, the fluid-structure-coupling poses a considerable challenge to detailed numerical modeling. A recently developed own numerical method capable of representing such a situation is applied, generating highly resolved transient data of fluid and structure motion. The talk will provide information about the numerical method and then focus on the analysis of the data highlighting the intricate coupling between the unsteady turbulent flow field and the flexible structures.

An isogeometric Mortar-Based Model for EHL contacts

Tong, Yan *(Institute of Dynamics and Vibrations, TU Braunschweig, Germany)*
Müller, Michael *(Institute of Dynamics and Vibrations, TU Braunschweig, Germany)*
Ostermeyer, Georg-Peter *(Institute of Dynamics and Vibrations, TU Braunschweig, Germany)*

15:20

Modeling the Elasto-Hydrodynamic Lubrication (EHL) contact in tribological systems remains a challenging problem due to the interaction of multiple physical fields including solid deformations and the multiphase fluid flow of the lubricant and cavitation bubbles. The complexity is further exacerbated by the fact that solid contacts can occur when the pressure build-up in lubricants cannot bear the external high load. To address these challenges, this paper presents a new model for the EHL contact that incorporates a combination of the mortar method and Non-Uniform Rational B-Splines (NURBS) based isogeometric analysis.

The new model employs the Reynolds equation for the lubricant flow and includes a mass-conserving cavitation algorithm, which allows for efficient simulation of the complex two-phase flow of the lubricant and cavitation bubbles. Large deformations of the solid bodies caused by the contact between the asperities and by the high fluid pressures are also considered in this model, making it a more comprehensive representation of the tribological system. Additionally, the model applies a frictional contact formulation using the Augmented-Lagrangian method, which couples the potential solid contacts into the system.

One of the key benefits of this new model is its ability to discretize the solid bodies and the fluid domain using inconsistent meshes, reducing the computational cost. This is important because finer meshes are usually required for the complex cavitation phenomena in the fluid domain, and this model makes it possible to handle these computations efficiently. Additionally, the model is capable of dealing with both stationary and transient EHL contacts, making it a powerful tool for understanding the basic mechanism of tribological systems under a wide range of conditions.

This new model offers a comprehensive representation of tribological systems by considering multiple physical fields, including solid deformations, multiphase fluid flow, and potential solid contacts. By incorporating advanced computational techniques such as the mortar method and the NURBS-based isogeometric analysis, this model is a valuable tool for researchers and engineers working in the field of tribology. By providing a more complete understanding of the basic mechanism of tribological systems, it can contribute to the development of more efficient and effective tribological solutions.

Towards coupled fire-structure simulations for forecasting smoke leakage in case of concrete structures under fire

Palani, Arulnambi *(Chair of Fluid Mechanics, Helmut Schmidt University/University of the Federal Armed Forces, Hamburg, Germany)*
Kandekar, Chaitanya *(Chair of Structural Analysis, Helmut Schmidt University/University of the Federal Armed Forces, Hamburg, Germany)*
Breuer, Michael *(Chair of Fluid Mechanics, Helmut Schmidt University/University of the Federal Armed Forces, Hamburg, Germany)*
Weber, Wolfgang E. *(Chair of Structural Analysis, Helmut Schmidt University/University of the Federal Armed Forces, Hamburg, Germany)*

15:40

Computational modeling of fire-structure interaction demands the coupling between several models typically implemented in independent simulation software describing distinct physical processes [1]. For instance, in the event of a fire breakout or building on fire, the fire not only increases the temperature of the immediate area but also initiates structural damage, leading to the spalling of the concrete along with the propagation of the smoke, heat, and radiation originating from the fire. As a result of the progressive structural damage caused by the fire such as macro cracks or breakthroughs in the wall, smoke and other hazardous gases begin to disperse or thrust into the previously unaffected zone. Thus, it represents a coupled multi-physics problem, which is not well addressed in the scientific community, yet. Therefore, the investigation of such fire-structure interactions requires a comprehensive computational modeling and simulation framework that couples the consequences of various phenomena with minimal invasive solver modifications. In this work, the structural model treats concrete as a multi-phase porous material exposed to high temperatures resulting from the fire. For this purpose, the structural solver is coupled with a computational fluid dynamics (CFD) solver to setup a computational framework for such fire-structure simulations. Herein, the combustion process of the fire and the smoke propagation is carried out using the open-source software denoted Fire Dynamics Simulator (FDS) [2] and the thermo-hydro-mechanical fracture is computed using a FEniCs-based solver. The finite-difference method based FDS solves the filtered Navier- Stokes equations using the large-eddy simulation (LES) technique to describe the turbulent flow and heat transfer including radiation and combustion inside the fluid domain. The concrete damage such as cracks, holes or spalling is computed using a phase-field method in a separate solver based on the thermal boundary conditions from the fluid simulation. Subsequently, both solvers are coupled using an open-source coupling framework. Based on the rate at which the crack or spalling is developing, the computational domain of the fluid solver has to be adapted taking the generated breakthroughs in the wall structure into account for the ongoing CFD simulation. It allows for the leakage of smoke gases through the concrete wall structure and thus the spreading of the fire scenario. The proposed model is illustrated by an example case that forecasts the leakage of smoke and hazardous gases from the damage caused by the thermal spalling induced on the concrete wall structure.

1. F. Pesavento, M. Pachera, B. A. Schrefler, D. Gawin and A. Witek, “Coupled numerical simulation of fire in tunnel”, AIP Conference Proceedings 1922, 090003, 2018.
2. K. Mcgrattan, S. Hostikka, J. Floyd, H. Baum, R. Rehm, W. Mell and R. Mcdermott, “Fire Dynamics Simulator Technical Reference Guide”, NIST Special Publication 1018, National In-

stitute of Standards and Technology, Gaithersburg, MD, 2012.

S07-05: Coupled problems

Date: June 1, 2023 08:30-10:30
Room: CHE/S89

Simulation of Powder Bed Fusion Processes using Smoothed Particle Hydrodynamics: Physical Modeling and Requirements on Meshfree Solution Schemes

Weißenfels, Christian *(University of Augsburg, Germany)* 08:30

The big promise of Additive Manufacturing is the rapid production of individualized components directly on-site and on-demand, which can be fabricated at the price of mass production. The speed of the manufacturing process, the quality and the reproducibility of a printed component still do not meet the requirements of industrial production. Numerical simulations enable the virtual reproduction of all physical phenomena during the printing stages. Thus, the key factors of 3D-printing can be analyzed directly on the computer. In addition, individual processes can be optimized virtually or new printing techniques can be developed. Meshfree methods, such as Smoothed Particle Hydrodynamics (SPH), can simulate large deformations and motions with free surfaces based on a Lagrangian description of the differential equations and thus represent ideal discretization schemes for the calculation of fusion processes occurring in Additive Manufacturing. In this talk, the physical processes that occur during powder bed fusion methods will be presented. In addition, the necessary conditions for spatial discretization schemes to ensure a good approximation of the true solution of the underlying differential equations will be presented concisely. The focus is especially on Smoothed Particle Hydrodynamics. This method has recently been increasingly used for the virtual reproduction of Additive Manufacturing processes. Finally, the numerical implementation is presented in order to be able to simulate the behavior of powder bed fusion processes on the particle scale. In addition, individual influencing factors, such as the modeling of the laser-material interaction, are analyzed numerically.

Grinding process model considering an intermediate liquid phase

Kästner, Felix *(RPTU, Germany)* 09:10
de Payrebrune, Kristin *(RPTU, Germany)*

In order to fulfill the increasing quality and precision requirements in industrial production, the manufacturing processes and methods have to be further optimized. Various approaches are being employed to achieve this. In the past, experimental test series and adjustments to the process, based on the test results, have proven successful for this purpose. Due to high-tech machinery and tools and more limited timeframes, it is becoming increasingly uneconomical to achieve this optimization by experimental approaches.

Furthermore, by far not all processes can be investigated by experimental investigations. Interactions in the microscopic range or even on the molecular level cannot be considered at all or only rudimentarily in this way. In order to address this problem, model-based analysis methods are constantly becoming more important in industrial use. This approach has

already been established for various manufacturing processes and has become a key technology in modern production.

However, the grinding process, which plays an essential part in precision manufacturing, cannot be fully modelled to the present day. This is also due to the fact that the process itself is not yet entirely understood. In this respect, the grinding process still reveals a lot of potential in terms of reliable predictions. In order to exploit this potential and to improve the understanding of the process itself, a physical grinding model is developed. This allows a wide range of manufacturing parameters to be tested and their effects predicted on the basis of numerical models. Here, process-typical influencing factors as well as commonly used cooling lubricants are considered. In this context, the link between the mechanical solid interactions and the liquid cooling lubricants is the central concern of the current development.

Modelling the post-buckling behaviour of steel sheets under induction heating

Filkin, Vladimir *(TU Wien, Vienna, Austria)*
Vetyukov, Yury *(TU Wien, Vienna, Austria)*
Toth, Florian *(TU Wien, Vienna, Austria)*

09:30

Induction heating is an important technology for many engineering applications. The main reason is that induction heating has several technical advantages over other methods, due to high power densities allowing rapid temperature increase, heat supplied directly within the target body, no contamination, etc. Designing induction heating systems requires accurate modelling of the magnetic field, temperature field and, in many cases, interaction effects: Joule losses from the induced eddy currents are source terms for the thermal problem [1]. Another significant interaction effect is the presence of mechanical deformations caused by thermal expansion. One needs to account for this effect to accurately describe the induction heating of thin steel sheets. Thermal expansion strongly affects the magnetic configuration since thin sheets are prone to thermal buckling, leading to large deformations. We suggest a modelling strategy combining a computationally highly efficient mechanical shell description for the thin sheet with a standard continuum model for eddy current and thermal problems through an iterative coupling algorithm. The problems are solved numerically using the finite element method. For magnetic and heat conduction models, we used open-source FEM software openCFS [2]. For the mechanical problem, we used an in-house solver. The solver is based on a Kirchoff-Love shell model built with the energy approach and the variational principle [3]. The necessary C^1 interelement continuous approximation of the geometry of the shell surface is achieved using 12 DoF in each of the four nodes of the element, namely the three components of the position vector, its first-order derivatives with respect to both local coordinates and the mixed second order derivative. This smooth approximation ensures rapid mesh convergence of the structural mechanics solution. We test the suggested computational procedure on simple models related to industrial applications and study the sensitivity of post-buckling behaviour with respect to various mechanical and electromagnetic parameters. The iterative method significantly increases the accuracy of post-buckling, thermal and magnetic modelling for a wide range of conditions. The proposed algorithm is the first step in exploiting the often unavoidable bucking positively, e.g. by accounting for the predicted steel sheet shape when evaluating thermal fields with higher accuracy.

[1] K. Roppert, F. Toth, and M. Kaltenbacher, “Simulating induction heating processes using harmonic balance FEM”, 2019.
[2] openCFS, https://opencfs.org/. [3] Y. Vetyukov, “Finite element modeling of Kirchhoff-Love shells as smooth material surfaces”, 2014.

Physics-Informed Reduced Order Modeling in Context of Digitial Shadows for Plastics Profile Extrusion

Hilger, Daniel *(CATS, RWTH Aachen University, Germany)* 09:50
Hosters, Norbert *(CATS, RWTH Aachen University, Germany)*

In many industries, the digitization of processes is still a major challenge. Especially when digitization is not just limited to the collection of arbitrary data, but even more so if this data should be used as direct feedback in the process itself. This type of digitized process is often referred to as digital shadow or digital twins. One component of digital shadows are often reduced order models (ROM) of conventional numerical methods. The ROM aspect accounts for the short evaluation times of the methods often demanded in the context of digital twins.

The process investigated in the course of the presented work is plastics profile extrusion, respectively only the cooling section of the process. In the cooling section, the still liquid but already formed material cools down until it solidifies. Here, the challenge is to cool the melt as uniformly as possible. Due to the high sensitivity of plastics, the extrudate would otherwise undergo undesired warpage and deformation effects. For this reason, a coupled model calculating the deformation based on the estimated temperature distribution is particularly valuable for the extrusion process. Based on those predictions, the extrudate cooling could be adapted to current production conditions to meet demanded product specifications.

We present a physics-informed [1] ROM for the prediction of temperature and deformation considering varying production conditions. The presented material model is based on the temperature-induced shrinkage model of Zwicke [2]. Therein, cooling induced temperature gradients cause internal stresses that finaly result in material deformation. Further, we will put the presented ROM in context of alternative ROM approaches and discuss its advantages and drawbacks.

Acknowledgment: Funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Germany’s Excellence Strategy-EXC-2023 Internet of Production-390621612.

[1] Raissi, M. , Perdikaris, P. , and Karniadakis, G.E. . Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations, Journal of Computational physics 378 (2019): 686-707.
[2] Zwicke, F Inverse shape design in injection molding based on the finite element method, Dissertation, Rheinisch-Westf alische Technische Hochschule Aachen, 2020.

Simulation of the laser metal deposition process using meshfree methods

Tang, Xiaofei *(Leibniz Universität Hannover, Germany)* 10:10
Weißenfels, Christian *(Universität Augsburg, Germany)*
Wriggers, Peter *(Leibniz Universität Hannover, Germany)*

The Laser Metal Deposition (LMD) as a process of additive manufacturing provides a highly accurate deposition of different materials at various locations and yields ideal adaptation for

the fabrication of functionally graded materials. The fact that LMD lacks reproducibility makes it difficult and costly for related research solely carried out by experiments. Furthermore, the slow speed for fabrication also inhibits scientific works on this subject. The Simulation of LMD Process by means of mesh-free method like incompressible Smoothed Particle Hydrodynamics (ISPH) serves an effective way to find out the relationship between structure, process and properties of LMD. It also provides a way for virtual design to improve the accuracy and efficiency of LMD process. Two sub-processes are included in this project: one is the simulation of powders falling along nozzles which is modeled by discrete-element-method (DEM). The other process that is also the main part of LMD is to simulate the molten powders depositing on the substrate by using ISPH. For the purpose of improving efficiency, the DEM process and SPH process are coupled by means of techniques of intercommunication. The fundamental physical concepts involved in the LMD process are surface tension, Wetting effect, recoil pressure, heat radiation, conduction and convection. Each of those needs to be modeled and integrated into the final simulation. In this work, the correctness of kernel function and its gradient is employed in order to rectify the errors caused by the truncation of the support from the kernel function. With this correctness, the multiple physical models become more compatible and yield a stable and reasonable result.

S07-06: Coupled problems

Date: June 1, 2023 16:00-19:00
Room: CHE/S89

A magneto-mechanically coupled material model for Barkhausen noise investigation

Dorn, Christian *(Kiel University, Germany)* 16:00
Wulfinghoff, Stephan *(Kiel University, Germany)*

To detect magnetic fields of heart and brain, we typically need high-performance magnetometers such as SQUIDs (superconducting quantum interference devices) or OPMs (optically pumped magnetometers). Since these magnetic field sensors are very complex and expensive, it is desirable to develop more accessible, easy-to-handle and cost-effective alternatives. One possible alternative are composite magnetoelectric thin film sensors. These sensors involve magnetostrictive and piezoelectric thin film materials and their operation is based on the interaction of multiple coupled fields. The magnetic field is translated into mechanical strain in the magnetostrictive material which is surface-coupled to the piezoelectric material. In the latter, the strain is translated into an electric signal.

One of the limiting factors of this sensor concept is magnetic noise. We are particularly interested in the noise caused by the interaction of domain walls with defects (Barkhausen noise). As the name suggests, magnetic noise is intrinsic to the magnetic material. Hence we focus on the magneto-mechanical part and omit the piezoelectric part. We model the micro-magneto-mechanical material behavior using the framework of generalized standard materials. The formulation includes exchange energy, anisotropy energy, demagnetizing energy and elastic energy as conservative contributions and a dissipative contribution in the form of a dissipation potential. The coupled problem encompasses magnetization, scalar magnetic potential and displacement degrees of freedom. We state the mechanical problem in the small strain setting where we assume an additive decomposition of strain into an elastic part, a magnetostrictive part and an eigenstrain contribution. In terms of the magnetic problem, we implement the restriction of magnetization to the unit sphere by means of the exponential map. To solve the coupled problem, we use the finite element method. Our computation scheme for Barkhausen noise is based on ensemble averaging over large sets of simulations with varying microstructures. We showcase numerical examples to illustrate our magneto-mechanically coupled material model and our noise computation scheme.

A note on NdFeB magnets generated by severe plastic deformation

Reichel, Maximilian *(Universität Duisburg-Essen, Germany)* 16:20
Schröder, Jörg *(Universität Duisburg-Essen, Germany)*

The renewable energy supply, the independence of fossil resources, as well as the change in mobility act as a driving force on technological innovation. To meet these challenges of our time, new and particularly powerful high-performance magnets are necessary [1], relying on new earth abundant materials and resource efficient processes. It has been shown that composite materials consisting of ferromagnetic grains separated by paramagnetic interphases can contribute to significant improvements in coercivity, when these interphases decouple

the magnetic exchange between the individual grains, compare [2]. Novel processing routes based on severe plastic deformations (SPD) or additive manufacturing (AM) can be an option to tailor such magnetic composites. Here, the micromagnetic theory can be applied to numerically predict the magnetization distributions on fine scales. Due to their flexibility, finite elements are well suited to discretize and analyze strongly heterogeneous microstructures [5]. The evolution of the magnetization vectors is described by the Landau-Lifshitz-Gilbert equation, which requires the numerically challenging preservation of the Euclidean norm of the magnetization vectors, see [4, 3]. With the aim to correctly reproduce the behavior of magnetic materials, competing energy contributions are considered within the energy functional, which are also responsible for the formation of magnetic domains. Also, grain boundaries, defect layers and misoriented grains can have a huge impact on the macroscopic hysteresis behavior of magnetic materials. Especially magnets formed by SPD are exposed to the potential stress-induced defects that might outweigh their production benefits. Hence, micromagnetics analyses are performed to estimate these risks and challenges of these novelties.

[1] O. Gutfleisch, M.A. Willard, E. Bruck, C.H. Chen, S.G. Sankar and J. Ping Liu. Magnetic Materials and Devices for the 21st Century: Stronger, Lighter, and More Energy Efficient. Advanced Materials, 23: 821-842, 2011.
[2] M. Soderžnick, H. Sepehri-Amin, T.T. Sasaki, T. Ohkubo, Y. Takada, T. Sato, Y. Kaneko, A. Kato, T. Schrefl and K. Hono. Magnetization reversal of exchange-coupled and exchange-decoupled Nd-Fe-B magnets observed by magneto-optical Kerr effect microscopy. Acta Materialia, 135: 68-76, 2017.
[3] A. Prohl. Computational Micromagnetism. Computational Material Science, 1st Edit., Springer, 2001.
[4] M. Reichel, B.-X. Xu and J. Schröder. A comparative study of finite element schemes for micromagnetic mechanically coupled simulation. Journal of Applied Physics, 132: 183903, 2022.
[5] A. Vansteenkiste, J. Leliaert, M. Dvornik, M. Helsen, F. Garcia-Sanchez

A thermo-chemo-mechanically coupled continuum theory and it's application in Finite-Element simulations

Gisy, Johannes *(Karlsruhe Institute of Technology (KIT), Germany)*
Dyck, Alexander *(Karlsruhe Institute of Technology (KIT), Germany)*
Böhlke, Thomas *(Karlsruhe Institute of Technology (KIT), Germany)*

16:40

Applications, which involve chemo-thermo-mechanically coupled processes gain more and more interest in the research community [1], e.g. for use cases like fuel cells or the conversion of excess electric power to hydrogen in an electrolysis when these technologies require higher temperatures. During the operation of solid oxide cells at high temperatures failure is detected as thermal and chemical processes induce mechanical tensions that lead to cracks [2]. To cope with the numerous challenges while developing these systems, appropriate continuum models for structure simulations are necessary.

Therefore, the aim of this talk is to derive a thermo-chemo-mechanically coupled theory for small deformations in a thermodynamic consistent setting. We start by presenting the necessary balance equations and derive the constitutive relations thermodynamically consistent, which lead to a set of fully coupled partial differential equations, that can be solved to describe chemical, thermal and mechanical effects. The basic fields being solved for are the

displacements, temperature and the chemical potential. The usage of the chemical potential simplifies the interpretation and application of boundary conditions at the cost of numerical difficulties later on.

An implementation of the coupled set of PDE's in ABAQUS is presented, making use of the user-defined-element subroutine. We derive all necessary residual equations and tangents analytically and use a fully implicit time stepping method. We close with an illustrative example, that points out some occurring effects of the fully coupling.

[1] Anand, L. (2011). A thermo-mechanically-coupled theory accounting for hydrogen diffusion and large elastic-viscoplastic deformations of metals. *International Journal of Solids and Structures*, *48*(6), 962-971.

[2] Lenser, C., Zhang, J., Russner, N., Weber, A., Guillon, O., & Menzler, N. H. (2022). Electro-chemo-mechanical analysis of a solid oxide cell based on doped ceria. *Journal of Power Sources*, *541*(February), 231505.

An efficient Finite Element approach for macroscopic boundary value problems of ferroelectric continua based on multiscale modeling

Wakili, Reschad *(University of Kassel, Germany)*
Lange, Stephan *(University of Kassel, Germany)*
Ricoeur, Andreas *(University of Kassel, Germany)*

17:00

Ferroelectric as well as ferromagnetic materials are widely used in smart structures and devices as actuators,sensors etc. Regarding their nonlinear behavior, a variety of models has been established in the past decades.Investigating hysteresis loops or electromechanical/magnetoelectric coupling effects, only simple boundary value problems (BVP) are considered. In [1] a new scale-bridging approach is introduced to investigate the polycrystalline ferroelectric behavior at a macroscopic material point (MMP) without any kind of discretization scheme, the so-called Condensed Method (CM). Besides classical ferroelectrics, other fields of application of the CM have been exploited, e.g. [2, 3, 4]. Since just the behavior at a MMP is represented by the CM, the method itself is unable to solve complex BVP, which is technically disadvantageous if a structure with e.g. notches or cracks shall be investigated.

In this paper, a concept is presented, which integrates the CM into a Finite Element (FE) environment. Considering the constitutive equations of a homogenized MMP in the weak formulation, the FE framework represents the polycrystalline behavior of the whole discretized structure, which finally enables the CM to handle arbitrary BVP. A more sophisticated approach completely decouples the constitutive evolution from the FE discretization, by introducing an independent material grid. Furthermore, energetic consistencies of scale transitions from grain to MMP and MMP to macroscale are investigated. Numerical examples are finally presented in order to verify the approach.

References

[1] Lange, S. and Ricoeur, A., A condensed microelectromechanical approach for modeling tetragonal ferroelectrics, International Journal of Solids and Structures 54, 2015, pp. 100 - 110.

[2] Lange, S. and Ricoeur, A., High cycle fatigue damage and life time prediction for tetragonal ferroelectrics under electromechanical loading, International Journal of Solids and Structures

80, 2016, pp. 181 - 192.
[3] Ricoeur, A. and Lange, S., Constitutive modeling of polycrystalline and multiphase ferroic materials based on a condensed approach, Archive of Applied Mechanics 89, 2019, pp. 973 - 994.
[4] Warkentin, A. and Ricoeur, A., A semi-analytical scale bridging approach towards polycrystalline ferroelectrics with mutual nonlinear caloric-electromechanical couplings, International Journal of Solids and Structures 200 - 201, 2020, pp. 286 - 296.

Computational and data-driven surrogate modeling of structural instabilities in electroactive polymers

Sriram, Siddharth *(Institute of Applied Mechanics (CE), University of Stuttgart, Germany)* 17:20
Polukhov, Elten *(Institute of Applied Mechanics (CE), University of Stuttgart, Germany)*
Keip, Marc-Andre *(Institute of Applied Mechanics (CE), University of Stuttgart, Germany)*

Dielectric elastomers (DEs), a class of incompressible electroactive polymers, are soft composites that deform mechanically under the action of an applied electric field. It is well known that under certain electro-mechanical loading conditions, DE specimens buckle resulting in inhomogeneous deformation on the structural level [1]. The objective of this work is to characterize the onset of such structural instabilities in DE film-substrate bilayers over a wide range of tunable geometrical and material properties by adopting a data-driven surrogate modeling approach. The required data is generated using a finite-element-based instability analysis framework, for which a saddle-point-based variational principle for electro-elastostatics, involving the deformation map and the scalar electric potential as the primary fields, is implemented [2]. In this setting, the onset of structural instability in the bilayer system corresponds to the signature change of the global indefinite tangent matrix, as shown in [3]. Within the considered design space for the DE bilayer, the data points are sampled by implementing the Sliced Latin Hypercube Design (SLHD) algorithm proposed in [4], which has been shown to ensure space-fillingness of the resulting sampled data points. Machine-learning-based surrogate models are then developed to predict the critical applied surface charge density for the onset of wrinkling instability and the resulting number of half walves on the surface of DE bilayers.

References:

[1] M. Bahreman, N. Arora, H. Darijani & S. Rudykh. Eur J Mech Solids, 2022.
[2] C. Miehe, D. Vallicotti & D. Zäh. Int J Numer Methods Eng, 102:1605-1637, 2015.
[3] J. Schröder, N. Viebahn, P. Wriggers, F. Auricchio & K. Steeger. Comput Mech, 2017.
[4] P. Qian. J Am Stat Assoc, 107:393-399, 2012.

Coupling of diffusional phase transformations and constitutive laws to predict damage at small scales

Flachberger, Wolfgang *(Montanuniversity Leoben, Austria)*
Gaddikere Nagaraja, Swaroop *(Montanuniversity Leoben, Austria)*
Antretter, Thomas *(Montanuniversity Leoben, Austria)*
Svoboda, Jiri *(Czech Academy of Sciences)*
Petersmann, Manuel *(Kompetenzzentrum für Automobil & Industrieelektronik, Austria)*
Scheiber, Daniel *(Material Center Leoben, Austria)*

17:40

This work presents a finite element variational formulation for the treatment of diffusional phase transformations using the Discontinuous Galerkin Finite Element Method (DGM). The diffusion model used is thermodynamically consistent and employs fundamental principles such as the vacancy mechanism of solid body diffusion. As Vacancies are a non-conserved quantity, their evolution is described by a type of transport equation, which is generally associated with fluid- rather than solid-mechanics. This is one of the reasons why the classical Galerkin Finite Element Method does not suffice for this type of model and the DGM needs to be employed. The model is characterized by sharp transitions between phases (sharp interface model) which is in strong contrast to other state of the art methods for describing diffusional phase transformations like the Phase Field Method (PFM). A binary system is studied whose behaviour is described by two differential equations which are solved by an implicit, fully coupled scheme. The diffusion model is used to predict both the phase growth as well as damage relevant phenomena such as trapping of components at grain boundaries and other imperfections. Furthermore, the diffusion is coupled with a constitutive model for the mechanical material behaviour. The coupling is done in both ways considering the influence of diffusion on mechanics via phase-dependent material parameters as well as by considering the influence of stresses and strains on the diffusion. This enables a detailed investigation of the many phenomena that are observed in metals at the small scales.

CT-data-based coupled poro-chemical modeling of transport in concrete

Meyer, Knut Andreas *(TU Braunschweig, Germany)*
Kruse, Roland *(TU Braunschweig, Germany)*
Jänicke, Ralf *(TU Braunschweig, Germany)*

18:00

High initial strength is not sufficient for durable reinforced concrete structures. The ability to remain strong when subjected to the environment over time is equally important. For example, many concrete constructions are subjected to chloride via seawater or salt-based deicing. The rebar corrodes in such environments unless protective or corrective methods prevent chloride intrusion. However, developing such methods requires physically motivated and well-calibrated models.

In this contribution, we develop such models. Specifically, we focus on formulating a model for ionic transport in partially saturated concrete, accounting for both the convective and diffusive parts. In contrast to common modeling approaches, we also consider how water- [1] and ion-binding [2] influence transport properties. These interactions play a crucial role in the chloride intrusion process.

Experiments, including in-situ Computer Tomography (CT), complement the numerical modeling. The CT data enable visualization of transport phenomena through the concrete microstructure with a resolution of 15 micrometers. This qualitative data motivates the model formulations. Furthermore, we obtain quantitative data, such as waterfront motion, for calibration and validation with differential imaging.

Our model can fit both experiments from the literature on anomalous transport [1], as well as our in-house experiments. A notable feature of the model is the modeling of water binding via evolution laws. This approach enables the extraction of relevant time scales from swelling experiments [3]. Furthermore, the formulation can be coupled to mechanical deformations to study the influence of impermeable aggregates embedded in the cement matrix.

References

[1] S. C. Taylor, W. D. Hoff, M. A. Wilson, and K. M. Green, "Anomalous water transport properties of Portland and blended cement-based materials," *J. Mater. Sci. Lett.*, vol. 18, no. 23, pp. 1925-1927, 1999, https://doi.org/10.1023/A:1006677014070.

[2] A. Ben Fraj, S. Bonnet, and A. Khelidj, "New approach for coupled chloride/moisture transport in non-saturated concrete with and without slag," *Constr. Build. Mater.*, vol. 35, pp. 761-771, 2012, https://doi.org/10.1016/j.conbuildmat.2012.04.106.

[3] N. M. Alderete, Y. A. Villagrán Zaccardi, and N. De Belie, "Physical evidence of swelling as the cause of anomalous capillary water uptake by cementitious materials," *Cem. Concr. Res.*, vol. 120, no. September 2018, pp. 256-266, 2019, https://doi.org/10.1016/j.cemconres.2019.04.001.

Effects of inhomogeneous heating on the unfolding of shape memory alloy fibers

Wolf, Sebastian *(University of Kassel, Germany)*
Descher, Stefan *(University of Kassel, Germany)*
Kuhl, Detlef *(University of Kassel, Germany)*

18:20

In recent years, ultra-high-performance concrete (highly dense concrete filled with steel fibers, UHPC) has proven itself as a material for load-bearing protective components and the implementation of efficient concrete structures due to its high strength, fire resistance and high energy dissipation. Recent works suggest using iron-based shape memory alloys as fiber material [1] to introduce an internal prestress state [2], or to boost fiber volume fraction [3]. The latter feature is focus of the present work. Its principle is a reduction of agglomeration that is strongly present when casting UHPC at higher volume fractions. This is achieved by rolling up the fibers, which reduces interactions. When the casting process is completed, the shape memory effect is activated, which straightens the SMA-fibers. The result is that fiber volume fractions significantly above the maximum values for standard UHPC are reachable. To predict the unfolding of fibers in the above-mentioned process is a multidisciplinary task. Since it is not energetically efficient to heat up large volumes of UHPC, it is intended to use inductive heating. Although the induced heat source is not evenly distributed over the fibers, it is very high at the surface and decreases towards the core. The penetration depth is strongly dependent on the frequency of the induced current. As the environment is fresh concrete, fluid-fiber interaction must be captured. Furthermore, the unfolding process is driven by an austenite-martensite transformation, which requires adequate modelling. Finally, unfolding

goes in hand with large deformations that need nonlinear numerical techniques. The present work deals with a simplified model that highlights the solid mechanical part of the overall process. It describes inductive heating in a simplified manner, nevertheless considering the inhomogeneous heat generation, and uses an empirical model to describe the one-way effect. Studies that highlight unfolding with respect to an uneven phase transformation over the fiber geometry are highlighted. Simulations are carried out using the nonlinear Finite-Element-Method [4] and Newmark [5] time integration.

References

[1] M. Schleiting, A. Wetzel, F. Gerland, T. Niendorf, O. Wünsch and B. Middendorf, RheoCon 2019, RILEM Books. 23, 142-148 (2020)

[2] S. Descher, P. Krooß, D. Kuhl, A. Wetzel and S. Wolf, PAMM 2022, 202200253 (2022)

[3] F. Gerland, A. Wetzel, T. Schomberg, O. Wünsch and B. Middendorf, Applied Rheology 29 (1), 130-140 (2019)

[4] M. A. Crisfield, Non-linear Finite Element Analysis of Solids and Structures, Volume 1, Wiley (1991)

[5] N. M. Newmark, Journal of the Engineering Mechanics Division 85 (3), 67-94 (1959)

FEM implementation of transient finite-strain coupled diffusion-deformation theories for hydrogels using Fenics

Urrea Quintero, Jorge Humberto *(Leibniz Universität Hannover, Institute of Mechanics and Computational Mechanics, Germany)*

Nackenhorst, Udo *(Leibniz Universität Hannover, Institute of Mechanics and Computational Mechanics, Germany)*

18:40

Hydrogels consist of a water-swollen and self-supporting polymeric network. They can undergo large deformations and permit the diffusion and release of molecules. Hydrogels have found applicability in various technical applications, especially in the food and biomedical fields. Modeling this type of material involves concurrent deformation of the polymer network and diffusion of the solvent through the network. In recent years, there has been a convergence towards a more complete coupled diffusion-deformation theory for describing the response of gels. Additionally, several methods related to the numerical implementation of these theories for solving coupled diffusion-deformation boundary value problems for gels have been published. The numerical implementation of most coupled theories using the finite element method (FEM) is often challenging because detailed numerical procedures and source codes are seldom published in scientific journal papers.

This contribution focuses on discussing the numerical implementation of large deformation coupled diffusion-deformation models for hydrogels in an open-source FEM package. We select some notable thermodynamically consistent models from the literature describing the mechanical response of hydrogels due to a solvent diffusion in the large deformation setting and compare their ability to describe the coupling mechanisms. The material models incorporate the effects of mechanical deformation and network swelling. We use the Fenics FEM package to solve these models in a variational monolithic way.

Our work includes benchmark tests on the absorption behavior of different hydrogel structures: transient swelling of a constrained hydrogel slab and free swelling of an initially square cross-section of unit side length.

The present work might impact the design of optimal protocols for hydrogel fabrication. For instance, the obtained outcomes are crucial when addressing tissue engineering scaffolds produced employing, e.g., 3D bioprinting technologies. The availability of a consistent framework to develop chemo-mechanical coupled computational models could help in the development of model-based industrial production with precise control over the manufacturing variables.

S07-07: Coupled problems

Date: June 2, 2023 08:30-10:30
Room: CHE/S89

Incremental variational principles for coupled chemo-mechanical problems in elastic and dissipative solids

Gaddikere Nagaraja, Swaroop *(Montanuniversitaet Leoben, Austria)* 08:30
Flachberger, Wolfgang *(Montanuniversitaet Leoben, Austria)*
Antretter, Thomas *(Montanuniversitaet Leoben, Austria)*

In this work, a variational framework for coupled chemo-mechanical problems in elastic and dissipative solids at infinitesimal strains is outlined. In doing so, it is seen that the gradient of the primary fields additionally enter the energetic and dissipative potential functions, resulting in additional balance equations. The governing balance equations of the coupled problem are derived as Euler equations of the incremental variational principles, formulated in a continuous-and discrete-time setting. Furthermore, the variables governing the inelastic process are locally condensed which yields a reduced global problem that is solved in a discrete-space-time setting. The symmetric structure of the proposed framework with respect to the primary and state variables is an advantage, and this is exploited in the numerical treatment within the finite element paradigm. The framework is applied to Cahn-Hilliard- type diffusion and Allen-Cahn-type phase transformation in elastic and elastic-plastic solids. The applicability of the proposed framework is demonstrated by means of two- and three-dimensional representative numerical simulations.

Influence of particle distribution on the quasistatic and dynamic mechanical properties of thermoplastic polyurethane magnetorheological elastomers

Kare Gowda, Darshan *(Technische Universität Dresden, Germany)* 08:50
Odenbach, Stefan *(Technische Universität Dresden, Germany)*

Thermoplastic magnetorheological elastomers (MRE) are a class of smart composite materials with multi-stimulated compliance. The embedded magnetic microparticles in the thermoplastic elastomer matrix enable the control of the mechanical properties of the composite by changing the temperature and external magnetic field. The understanding of the influence of different stimulating parameters on the mechanical properties of the MRE provides further insights into the influence of particle distribution in the MRE.

Cylindrical rod-shaped isotropic and anisotropic thermoplastic polyurethane magnetorheological elastomer (TPU-MRE) samples were prepared with 40 wt.% of iron microparticles. The samples were investigated for mechanical and microstructural properties. Quasistatic tensile and torsion tests followed by dynamic oscillation tests under different temperatures without and with a magnetic field with a flux density of 250 mT were performed. These tests allow to calculate the magnetorheological effect (MR effect), that is the difference in modulus of the material as a function of the magnetic field at different temperatures. For example, the MR effect for the tensile test is given as MR effect=$(E_B\text{-}E_O)/E_B$, where E_0 is Young's modulus of the sample without magnetization and E_B is Young's modulus of the sample at a magnetization of B = 250 mT.

The results reveal that the magnetorheological effect increases with the increase in temperature, and it is significantly more in the case of anisotropic samples compared to isotropic samples. This proves the influence of the stimulating parameters on the TPU-MRE on a macroscopic scale. To better understand the reasons behind these macroscopic changes, microstructural investigations of the samples were done using X-ray microtomography by subjecting the samples to similar stimulating parameters. The structure and distribution of particles were analysed using digital image processing. The pair correlation function offers a suitable method to examine the structure of the particles based on their distribution. This way we can correlate the material behavior such as the stiffening effect in a magnetic field to the changes in the inner microstructure of the material.

Financial support by DFG (Grant No. OD18/28-1) within SPP2100 is gratefully acknowledged.

Latent Heat Effects in Inductive Heating of Shape Memory Alloy Fibers

Descher, Stefan *(Institute of Structural Mechanics, University of Kassel, Germany)* 09:10
Krooß, Philipp *(Institute of Materials Engineering, Metallic Materials, University of Kassel)*
Kuhl, Detlef *(Institute of Structural Mechanics, University of Kassel, Germany)*
Wolf, Sebastian *(Institute of Structural Mechanics, University of Kassel, Germany)*

Ultra High Performance Concrete is highly dense concrete filled with steel fibers, and well known for its outstanding mechanical behavior in the civil engineering community. Further improvement is possible using pre-stretched shape memory alloy fibers instead. [1] They enable introducing an internal prestress state by activation of the one-way effect, which leads to fiber contraction. As a result, there is tension in the fiber, and largely compression in its proximity if the fiber geometry is chosen properly. [2] For activation, the fibers need to be heated up until a microstructure transformation from martensite to austenite takes place. Because heating up large parts is not energy efficient, this is done by an induction heater. [3] The present work deals with the efficiency of the inductive heating in the above described process. It considers the endothermic character of the martensite-austenite transformation, geometric and electromagnetic parameters, as well as an elastomeric fiber coating. The non-isothermal phase transition is modeled empirically, based on data from Differential Scanning Calorimetry. Parameter studies are performed for an axisymmetric single fiber case with an induction coil using the Finite-Element-Method.

[1] M. Vollmer, A. Bauer, J.-M. Frenck, P. Krooß, A. Wetzel, B. Middendorf, E. Fehling and T. Niendorf: Novel prestressing applications in civil engineering structures enabled by Fe-Mn-Al-Ni shape memory alloys, Engineering Structures 241, 112430 (2021).
[2] S. Descher, P. Krooß, D. Kuhl, A. Wetzel and S. Wolf: Internal prestressing of ultra-high performance concrete using shape memory fibers, PAMM 2022, 202200253 (2022, accepted for publication).
[3] T. Gleim, D. Kuhl, M. Schleiting, A. Wetzel and B. Middendorf: High-Order Numerical Methods for the Thermal Activation of SMA Fibers, PAMM 2019, 201900025 (2019)

Meso-scale thermo-magneto-mechanical constitutive model for magneto-active elastomers

Klausler, Will *(Technische Universität Dresden, Germany)* 09:30
Kaliske, Michael *(Technische Universität Dresden, Germany)*

Magneto-active elastomers (MAE) are one of many emerging smart materials. They have applications in mechanical, civil, and biomedical engineering as actuators, such as grippers, and dampers, such as tunable vibration absorbers. MAE consist of a soft polymeric matrix filled with micron-sized magnetizable particles. Set in a magnetic field, the particles displace, stiffening the entire composite by up to three orders of magnitude.

The literature contains myriad purely magneto-mechanical models for MAE. This contribution introduces a thermal component to enable prediction of heat generation in the composite due to oscillatory, visco-elastic mechanical deformations. This model, formulated for three-dimensional finite deformations, is capable of accurately modeling the behavior of incompressible materials through a Q1P0 finite element framework. Numerical simulations qualitatively show the capabilities of this model to describe the fully-coupled thermo-magneto-mechanical response of MAE. Simulations are also performed to fit model parameters to some experimental data. The semi-structured finite element mesh is generated exclusively with hexahedra.

Modeling and simulation of a dielectric elastomer sensor and of the substitute system of a sensor-integrated jaw coupling

Menning, Johannes Dieter Martin *(Institute of Solid Mechanics, Technische Universität Dresden, George-Bähr-Str. 3c, 01069 Dresden)* 09:50
Ewert, Arthur *(Institute of Machine Elements and Machine Design, Technische Universität Dresden, Münchner Platz 3, 01069 Dresden)*
Prokopchuk, Artem *(Institute for Semiconductors and Microsystems, Technische Universität Dresden, Nöthnitzer Straße 64, 01069 Dresden)*
Schlecht, Berthold *(Institute of Machine Elements and Machine Design, Technische Universität Dresden, Münchner Platz 3, 01069 Dresden)*
Henke, Markus *(Institute for Semiconductors and Microsystems, Technische Universität Dresden, Nöthnitzer Straße 64, 01069 Dresden)*
Wallmersperger, Thomas *(Institute of Solid Mechanics, Technische Universität Dresden, George-Bähr-Str. 3c, 01069 Dresden)*

With the advent of industry 4.0, the desire for machine elements to become smart is substantial. There are solutions where machine elements such as couplings comprise external sensors. However, these sensors change the overall required space for the coupling, which is often not desired. The aim of the current work is to present a substitute system for a sensor-integrated jaw coupling in which a dielectric elastomer sensor (DES) is integrated into the teeth of the elastic gear rim. During use of the coupling, the teeth of the gear rim are compressed, which leads to a deformation of the teeth and thus of the integrated DES, resulting in an increase in capacity. The applied torque can be derived from this increase in capacity of the DES. With the substitute system, different configurations of the sensor can be tested in order to find a good compromise between sensor size and sensitivity. The substitute system

is composed of (i) the material of the gear rim, thermoplastic polyurethane (TPU), (ii) the dielectric elastomer sensor and (iii) two strain amplifiers. All three components have the shape of cylinders, resp. of a hollow cylinder for the TPU. For this system, a finite element (FE) analysis is carried out, in which the mechanical response of the system for uniaxial compression is modeled. Due to the load, the sensor and also the dielectric layers will deform. The resulting change in capacitance due to the deformation of the sensor is investigated both analytically and numerically. For the analytical calculation, the current heights of the dielectric layers are determined and inserted into the analytical equation for a parallel plate capacitor. For the numerical calculation, the electrostatic field equations are solved on the deformed configurations of the equivalent system. For this purpose, alternating positive and negative electric potentials are applied to the electrodes. The capacity can then be determined by comparing the resulting internal energies. Finally, in the present research, we implement the sensor that has proven to be most suitable into a finite element model of a jaw coupling.

Modeling approaches for phase transition in growing Antarctic Sea Ice

Thom, Andrea *(ISD, University of Stuttgart, Germany)* 10:10
Ricken, Tim *(ISD, University of Stuttgart, Germany)*
Thoms, Silke *(AWI, Bremerhaven, Germany)*
Kutschan, Bernd *(AWI, Bremerhaven, Germany)*

Sea ice has a strong influence on the global climate linking the exchange of energy and gases between the atmosphere and the ocean. Changes in sea ice may also have a biologically respond concerning the ocean´s ecosystem structure and function as it constitutes a natural habitat and shelter for microorganisms and phytoplankton. Physical and mechanical changes in the properties of the sea ice structure may have an impact on the future Southern Ocean biological pump.

Seawater is trapped in so-called brine pockets during the growth of sea ice, providing a suitable environment for sea ice microorganisms. The microorganisms are supplied with nutrients from the seawater they need for primary production. A small-scale modelling of the porosity of the sea ice and its inclusions and the solid/brine multiphase microstructure, respectively, thermodynamics of air-sea interactions as well as sea ice-biological linkages is a necessary tool to understand the heterogeneous sea ice nature better.

A modular developed model based on the continuum mechanical description for multi-phase materials containing individual components, the extended Theory of Porous Media (eTPM), is presented. The model set up for the homogenized pancake ice structure captures all essential aspects of freezing and melting in connection with deformation, salinity profiles and brine transport via coupled partial differential equations (PDEs), which are solved with the Finite Element Method (FEM).

Focus in this contribution is on the different modeling approaches to describe the phase transition between salty sea ice water and the freezing sea ice. The physical basis is modeled on the one hand with a phenomenological approach on the macro-scale driven by the divergence of heat flux, see [1], and on the other hand by a phase-field model approach [2] implemented on the Gauss point scale.

[1] J. Bluhm, W. M. Bloßfeld, and T. Ricken. “Energetic effects during phase transition under freezing-thawing load in porous media-a continuum multiphase description and FE-simulation.” *ZAMM-Journal of Applied Mathematics and Mechanics/* 94.7-8 (2014): 586-608.
[2] K. Morawetz, S. Thoms, and B. Kutschan. “Formation of brine channels in sea ice.” *The European Physical Journal E* 40 (2017): 1-7.

S07-08: Coupled problems

Date: June 2, 2023 11:00-13:00
Room: CHE/S89

Numerically robust mixed finite elements for analyses of flexoelectricity

Serrao, Prince Henry *(Ruhr University Bochum, Germany)* 11:00
Kozinov, Sergey *(Ruhr University Bochum, Germany)*

Higher-order electromechanical coupling between mechanical strain gradients and an electric field is referred to as direct flexoelectricity, while coupling between electric field gradients and mechanical strains is known as converse flexoelectricity. Unlike piezoelectricity, even centrosymmetric dielectrics possess inherent flexoelectric properties due to the application of strain gradients. Piezoelectric materials, when considered at the nano- or micro-scale, acquire an additional flexoelectric contribution as a result of the non-homogeneous strain distribution. This makes flexoelectricity a suitable successor to piezoelectricity in small-scale devices such as nano- and micrometer MEMS. Consideration of both linear piezoelectric together with higher-order flexoelectric electromechanical coupling requires fully coupled electromechanical formulations. Classical continuum theories are unable to model the strain gradient effect. Toupin and Mindlin [1] were the first to extensively extended the higher-order theories proposed by Cosserat. However, such formulations require C^1-continuity due to the fourth-order partial differential equations. Mixed FEM formulations with C^0-continuity are actively used to circumvent this difficulty. Here, the displacements and their gradients are considered as independent quantities [2]. The numerical instability of the known mixed finite elements is inherent due to their dependence on the stabilization parameter. Recently, a computationally efficient second-order collocation-based mixed FE was proposed by the authors [3]. At the same time, two new user elements *Qu2s2p2l0* and *Qu2s2p2l1* were developed and implemented for classical mixed FEM. These elements are numerically robust without relying on stabilization parameters [4]. The advantage of these elements was verified on several existing mixed FE benchmark problems for flexoelectricity in dielectric solids, such as a plate with a hole and a thick cylinder. Additionally, a cantilever beam and truncated pyramid problems were calculated using mixed FE with piezoelectricity activated. The obtained results are crucial to investigate the intrinsic coupling of flexoelectric and piezoelectric effects.

References

[1] R. D. Mindlin, “Micro-structure in linear elasticity (1964),” *Arch. Rational Mech. Anal.*, 16 (1), 51–78, 1964.

[2] F. Deng, Q. Deng, W. Yu and S. Shen, “Mixed Finite Elements for Flexoelectric Solids,” *Journal of Applied Mechanics*, 84 (8), 081004, 2017.

[3] K. Tannhäuser, P. H. Serrao and S. Kozinov, “Second-Order Collocation-Based Mixed FEM for Flexoelectric Solids,” *Solids,* Special Issue “*Recent Advance in Ferroelectric composites*”, 4 (1), 39-70, 2023.

[4] P. H. Serrao and S. Kozinov, “Numerically robust C^0-continuous mixed FE for analyses of size-dependent flexoelectricity in piezoelectric solids”, *submitted, 2023*.

Theoretical investigation and analysis on ferroelectric energy harvesting cycles exploiting domain switching

Warkentin, Andreas *(Universität Kassel, Germany)* 11:20
Behlen, Lennart *(Universität Kassel, Germany)*
Ricoeur, Andreas *(Universität Kassel, Germany)*

Ferroelectrics exhibit many interesting effects, both linear and nonlinear, which is why these materials are widely used in science and industry. Recently, nonlinear effects have also been employed in the field of energy harvesting [1, 2, 3], while for a long time, only linear effects were exploited. Moreover, nonlinear effects are irreversible and are accompanied by energy dissipation, which generally leads to a temperature rise of the material. For modeling the characteristic nonlinear effects of ferroelectric materials, there are various possibilities, in particular microphysical and, phenomenological models. Ferroelectric energy harvesting concepts are investigated theoretically, based on a microphysically motivated thermo-electromechanical multiscale constitutive framework. Taking advantage of comparatively large changes of strain and polarization due to domain switching, the electric output is higher compared to what is commonly known as piezoelectric energy harvesting. Dissipative self-heating and augmented damage accumulation, on the other hand, may impede the operability of the harvesting device, in particular, if tensile stress is required for depolarization, as suggested by recent works [3, 1]. A new harvesting cycle [1] thus dispenses with tensile stresses and instead exploits the potential of existing residual stresses. It is further investigated to which extent a bias field, commonly applied to support repolarization as an important stage of the cycle, can be omitted, saving considerable effort on the technical implementation. Process parameters are obtained from various simulations by pareto-optimization, considering, inter alia, the effect of ambient temperature.

[1] A. Warkentin, L. Behlen and A. Ricoeur, Smart Mater. Struct. 10.1088/1361-665X/acafba (2023).
[2] L. Behlen, A. Warkentin and A. Ricoeur, Smart Mater. Struct. 30 035031 (2021).
[3] W. Kang, L. Chang and J. E. Huber, Nano Energy 93 (2022), p. 106862.

Towards modeling of concrete degradation caused by freezing-thawing cycles

Levent, Aykut *(Technische Universität Braunschweig, Germany)* 11:40
Meyer, Knut Andreas *(Technische Universität Braunschweig, Germany)*
Jänicke, Ralf *(Technische Universität Braunschweig, Germany)*

Freezing-thawing cycles can severely reduce durability and service life of porous construction materials, such as concrete, in cold climates. In moist environments, concrete absorbs water. Freezing and thawing then lead to expansion and shrinkage, causing internal stresses. Understanding this loading requires a multiphysics model that considers the hygro-thermo-mechanical interactions [1-2]. In this study, such a poromechanical model is created, which includes solid mortar, water and ice as constituents. As a first step, pores are considered fully saturated. Thus, the proposed model has three coupled fields; solid displacements, liquid pressure and temperature. To model freezing process, we adopt the assumption from [3] that the freezing temperature depends on the pore size, resulting in a gradual freezing-thawing in accordance with experimental evidence [3]. Experimental data is gathered by using X-

ray computed tomography (CT) to scan saturated concrete samples while applying heating and cooling cycles within the range of ±20°C. This method makes it possible to observe the initiation and progression of cracks. Our goal is to incorporate these fracture processes into the model and validate it through in-situ experiments.

[1] W. Zhou, C. Zhao, X. Liu, X. Chang, C. Feng, "Mesoscopic simulation of thermo-mechanical behaviors in concrete under frost action", Construction and Building Materials 157, (2017), 117-131.
[2] D. Eriksson, T. Gasch, R. Malm and A. Ansell, "Freezing of partially saturated air-entrained concrete: A multiphase description of the hygro-thermo-mechanical behavior", International Journal of Solids and Structures 152-153, (2018), 294-304.
[3] O. Coussy, P. J.M. Monteiro, "Poroelastic model for concrete exposed to freezing temperatures", Cement and Concrete Research 38, (2008), 40-48.

Variational Thermomechanical Reduced-Order Modeling of Shape Memory Alloy based Bistable Microactuators

Shamim, Muhammad Babar *(CAU Kiel, Germany)*
Hörsting, Marian *(CAU Kiel, Germany)*
Wulfinghoff, Stephan *(CAU Kiel, Germany)*

12:00

Parametric study for large scale non-linear material models using Finite element method (FEM) is computationally demanding due to strong non-linear material behavior and higher degrees of freedom. This study develops a thermomechanical model for a shape memory alloy-based microactuator that operates through thermal loading by Joule heating. The formulation is carried in generalized standard material (GSM) framework with the incorporation of thermomechanics. The reduced basis is captured from a pre-computed FEM model using proper orthogonal decomposition (POD). The optimization of the incremental thermomechanical potential computes the modal coefficients, and the reduced-order model is compared with a full-scale FEM model. The comparison demonstrates a low error rate of 0.973% for the displacement and 0.089% for the temperature, with an increase in computational speed of 9.56 times. The reduced-order model is tested on single and cooperative beam-like actuators, and the cross-coupling effects and bistability of the microactuators are explored.

On the coupled theory of thermoelasticity for nanoporous materials with triple porosity

Svanadze, Merab *(Ilia State University, Georgia)*

12:20

Prediction of mechanical properties of nanoporous materials is one of the current topics of continuum mechanics. According to the classical definition, such materials include those porous bodies whose pore diameter is in the range of 1-100 nm. In the present work, the linear mathematical model of thermoelasticity for nanomaterials with triple porosity is presented in which the coupled phenomenon of the concepts of Darcy's law and the volume fractions of three levels of pores (macro-, meso- and micropores) is proposed. Then, the 3D basic boundary value problems (BVPs) of this theory are investigated. Namely, the fundamental solution of the governing system of steady vibration equations in the considered theory is constructed explicitly. The Green's formulae are obtained and the uniqueness theorems for

classical solutions of the BVPs are proved. The basic properties of surface and volume potentials in the 3D linear coupled theory of thermoelasticity for materials with triple porosity are established. The existence theorems for classical solutions of the BVPs of steady vibrations in this theory are proved by using the boundary integral equations method and the theory of the singular integral equations. **Acknowledgments.** This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [Project # STEM-22-557].

Modelling of mechanically-induced failure processes in electrically conducting interfaces

Kaiser, Tobias *(Institute of Mechanics, TU Dortmund University, Germany; Mechanics of Materials Group, Eindhoven University of Technology, The Netherlands)*
Andreas, Menzel *(Institute of Mechanics, TU Dortmund University, Germany; Division of Solid Mechanics, Lund University, Sweden)*

12:40

Material interfaces occur at various length scales and may exhibit significantly different properties than the surrounding continuum. They have been in the focus of intense research since the pioneering works on material failure by Barenblatt and Dugdale from the early 60s and the studies on interface elasticity by Gurtin and Murdoch from the 70s. Both types of formulations have in common that the physical interface of finite thickness is not geometrically resolved but rather approximated as a lower-dimensional object. Moreover, it has recently been shown that both formulations can be regarded as limit cases of the unifying theory of general imperfect interfaces.

Motivated by the influence of grain boundaries and microcracks on the effective electrical properties of a material system, the present contribution focuses on the fundamentals of electro-mechanically coupled cohesive zone formulations for electrical conductors [1]. In the spirit of Barenblatt and Dugdale, it is assumed at the outset of the developments that the displacement-type fields may exhibit jump discontinuities across the interface, whereas the traction-type fields are continuous. For the electrical subproblem, this means that jumps in the electric potential field may occur, whereas the (normal projection of the) current density vector is continuous across the interface. In particular, it is shown that the continuity equation for the electric charge and Faraday's law of induction naturally give rise to non-standard jump conditions at the interface. In addition, coupling to thermal problems is established via a generalised form of the balance equation of energy and the dissipation inequality is studied so as to reveal thermodynamic restrictions.

The electro-mechanically coupled formulation is implemented into a multifield finite element code and representative boundary value problems that focus on the influence of mechanically-induced degradation processes on the electric conductivity of material interfaces are studied.

[1] Kaiser T., Menzel A. (2021) *Fundamentals of electro-mechanically coupled cohesive zone formulations for electrical conductors*. Comput Mech 68:51-67

S07-09: Coupled problems

Date: June 2, 2023 11:00-13:00
Room: CHE/183

A fully coupled chemo-mechanical phase-field model for reactive multi-component and multi-phase systems

Seupel, Andreas *(TU Bergakademie Freiberg, Germany)* 11:00
Roth, Stephan *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*

Modeling of the mechanical behavior of materials under the simultaneous consideration of phase transitions, diffusion and, chemical reaction processes is increasingly becoming the focus of current research [1-3]. Particularly, the coupling of these phenomena to mechanics has recently been studied [1,2].

We present a chemo-mechanical approach which is based on a mixture theory for multiple components and phases [2,3] within the framework of the non-equilibrium thermodynamics of internal state variables. Concerning the mechanics, a small strain setting is firstly considered, where the field coupling is established by concentration dependent swelling deformations, Bain strains related to phase transformations as well as phase dependent elastic properties. The influence of phase boundaries is introduced in a diffuse interface sense by the phase-field approach, more specifically, the energetic contributions of interfaces are included in the state potential via gradient contributions of the component mass fractions as well as order parameters representing different phases. The constitutive relations and the additional field equations of generalized Cahn-Hilliard and Allen-Cahn type are derived from a local entropy balance under the assumption of a localized Gibbs fundamental equation.

For the numerical solution of specific boundary value problems, a special finite element formulation is used. To this end, the field equations are recast into a mixed variational formulation [3], which allows field variable discretizations with low-order ansatz functions. A verification of the FE implementation is performed by means of benchmark problems for binary systems whose equilibrium solutions are known.

[1] Bai, Y.; Mianroodi, J. R.; Ma, Y.; da Silva, A. K.; Svendsen, B., Raabe, D.: Chemo-mechanical phase-field modeling of iron oxide reduction with hydrogen, *Acta Mater. (*2022), 231, 117899
[2] Svendsen, B.; Shanthraj, P.; Raabe, D.: Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids, *J. Mech. Phys. Solids (*2018) 112:619-636
[3] Seupel, A.; Roth, S., Kiefer, B.: Phase-field modeling of chemically reactive multi component and multi-phase systems, *PAMM(*2023), https://doi.org/10.1002/pamm.202200154
[4] Miehe, C.; Hildebrand, F. E.; Böger, L.: Mixed variational potentials and inherent symmetries of the Cahn-Hilliard theory of diffusive phase separation, *Proc. R. Soc. A (*2014) 470:20-130641

A phase-field model of elastic surfaces in flow

Kloppe, Maximilian *(TU Bergakademie Freiberg, Germany)* 11:20
Aland, Sebastian *(TU Bergakademie Freiberg, Germany; HTW Dresden, Germany)*

The small thickness of membranes, shells and capsules enables their efficient approximation as hyper-surfaces. Phase-field modeling provides a versatile tool to capture the motion of such elastic hyper-surfaces in fluid flow under bending and surface tension forces. However, the in-plane stretching of the surface has been widely neglected or approximated by inextensibility of the material.

In this talk, we develop a novel phase-field model for elastic hyper-surfaces in Navier-Stokes fluids, which includes bending, tension, and in-plane stretching. The model is based on a coupling of a phase-field model for two-phase flow to a fully Eulerian description of the surface deformation tensor. We apply the method to microfluidic experiments on lipid vesicles and illustrate how the results can be used to better understand the mechanical properties of cell membranes.

Phase field approximation of hyperelastic interfaces

Wilbuer, Hendrik *(Institute of Mechanics, TU Dortmund University, Germany)* 11:40
Mosler, Jörn *(Institute of Mechanics, TU Dortmund University, Germany)*

Phase field modeling has been successfully applied in a wide variety of applications and research areas, e.g. in fracture/damage mechanics as well as in the field of microstructure evolution. Within the present work, an extended model with focus on microstructure evolution is introduced. In contrast to previous works, deformation-dependent interface energies are considered. To be more precise, the hyperelastic interface energy depends on the (surface)deformation gradient. The final model is implemented into a mechanically coupled finite element environment and numerical simulations highlight the predictive capabilities of the resulting framework. Particularly, the effect of deformation-dependent energies is demonstrated.

Phase-field modeling of hysteretic behavior of shape memory alloys incorporating rate-independent dissipation

El Khatib, Omar *(TU Bergakademie Freiberg, Germany)* 12:00
von Oertzen, Vincent *(TU Bergakademie Freiberg, Germany)*
Patil, Siddhi Avinash *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*

Shape memory alloys (SMA) belong to a prominent class of mulitfunctional materials providing a variety of widely applicable engineering functionalities. Their uniqueness stems in part from their property of fully recoverable superelastic strains by simultaneously dissipating energy under stress and temperature controlled loading scenarios, which makes them very attractive for civil engineering applications (e.g. pre-stressing of concrete, protecting components against seismic events, etc.). Moreover, underlying microstructural evolution mechanisms involving phase-transformations between austenite and multi-variant martensite determine the characteristic behavior of these alloys and thus need to be adequately modeled on multiple scales. Despite numerous important contributions addressing the continuum mechanical description of SMA at the material point level—see [1,2] and the references

therein—the field of spatially regularized approaches is still heavily investigated. Accordingly, the phase-field method has manifested itself as an appropriate modeling framework resolving the evolution of complex interface topologies as observed in phase-transforming solids. However, the majority of existing phase-field models typically relies on rate-dependent formulations and thus remains incapable of reproducing quasi-static thermoelastic hysteresis behavior. In this regard, we propose a thermo-mechanically coupled and variationally consistent Allen-Cahn based phase-field approach, incorporating both rate-dependent and -independent dissipation potentials, as introduced in [3]. Involving local energetic minima continuously distributed within the range of SMA-specific transformation temperatures, the outlined framework is designed to account for sigmoidal type undercooling hysteresis as well as stress- and temperature-induced martensite pattern formation. The calibration of model specific parameters is shown to be directly related to experimentally observed austenite-martensite start and finish temperatures. Accordingly, the influence of driving force related threshold values on macroscopic hysteresis curves is investigated within finite element simulations of microstructure formation for different SMA. In addition, theoretical extensions of the proposed model towards multi-phase and multi-variant alloy systems are outlined in order to demonstrate its generalizability.

References:

[1] Lagoudas D. C, *Shape memory alloys: modeling and engineering applications*. Springer Science & Business Media, 2008.

[2] L. Xu, T. Baxevanis and D. C. Lagoudas, 2019. *A three-dimensional constitutive model for the martensitic transformation in polycrystalline shape memory alloys under large deformation*, Smart Mater. Struct. 28(7), 074004.

[3] K. Tuma, S. Stupkiewicz and H. Petryk 2018. *Rate-independent dissipation in phasefield modelling of displacive transformations*, J. Mech. Phys. Solids 114, 117-142.

Simulation of vibrating droplets using a phase field approach

Wolf, Jana *(Institute for Applied Mechanics, RPTU Kaiserslautern-Landau, Germany)* 12:20
Rutz, Xenia *(Institute for Applied Mechanics, RPTU Kaiserslautern-Landau, Germany)*
Stephan, Simon *(Laboratory of Engineering Thermodynamics, RPTU Kaiserslautern-Landau, Germany)*
Hasse, Hans *(Laboratory of Engineering Thermodynamics, RPTU Kaiserslautern-Landau, Germany)*
Müller, Ralf *(Division of Continuum Mechanics, TU Darmstadt, Germany)*

Droplet vibration is an important phenomenon in many technical applications. Correctly predicting the occurring behavior such as droplet detachment is a challenge for numerical simulations.

In this work, a so-called Navier-Stokes-Korteweg model that couples a gas-liquid phase field to the Navier-Stokes equations [1,2] is used to simulate a droplet on a horizontally vibrating surface. The influence of important modeling parameters as the static contact angle, the vibration frequency and the droplet size on the resulting droplet behavior is discussed and different choices for the boundary conditions are compared.

[1] H. Gomez, K. G. van der Zee. Computational phase-field modeling. In E. Stein, R. de Borst, & T. J. Hughes (Eds.), Encyclopedia of Computational Mechanics, Second Edition. John Wiley & Sons, Ltd (2017).
[2] F. Diewald, M. Heier, M. Horsch, C. Kuhn, K. Langenbach, H. Hasse, and R. Müller, J. Chem. Phys. 149, 064701 (2018)

S07-10: Coupled problems

Date: June 2, 2023 16:00-18:00
Room: CHE/S89

A numerical study of microbubble dynamics using the isogeometric boundary element method

Rajski, Michal Pawel *(Department of Continuum Mechanics, RWTH Aachen University, Germany)* 16:00
Itskov, Mikhail *(Department of Continuum Mechanics, RWTH Aachen University, Germany)*
Sauer, Roger Andrew *(Aachen Institute for Advanced Study in Computational Engineering Science (AICES), RWTH Aachen University; Faculty of Civil and Environmental Engineering, Gdansk University of Technology; Department of Mechanical Engineering, Indian Institute of Technology Kampur)*
Khiêm, Vu Ngoc *(Department of Continuum Mechanics, RWTH Aachen University, Germany)*

Cavitation describes the development of the vapor cavities or bubbles in a moving liquid due to a sudden drop in the pressure. The dynamics of the bubble and the cavitation process have been studied in the literature for a long time. From an engineering point of view, the main areas of interest revolve around the interaction between the bubbles and the rigid structures. Examples of this application are the simulation of underwater explosions, the influence of cavitation on the longevity of the ship propellers, fluid pumps and machines. In this work, we focus on the dynamics of microbubbles induced by the ultrasound waves for biomedical applications. Due to the small size of the microbubbles compared to the wavelength as well as the short time scales, the bubble dynamics can be modeled by an incompressible, inviscid and irrotational flow. This type of fluid behavior can be represented by potential theory and solved using the boundary element method (BEM). The advantage of using the BEM is that the influence of the fluid on the microbubble is solved based on the surface discretization only. The time evolution of the potential on the surface of the microbubble is described by the Bernoulli equation. The influence of an incident wave coming from the far-field can be captured using the matched asymptotic expansions analytically [1]. Together all mentioned approaches create a very interesting coupled framework able to capture the behavior of the complex problem using only surface discretization. To further improve the considered coupled framework, isogeometric analysis is used to represent the surface of the bubble [2]. The advantage of this type of discretization is that it is able to represent conic sections (such as circles, ellipses, spheres) exactly with a relatively small number of elements. This improves the accuracy of the BEM solution as well as increases the efficiency of the method. To further improve the quality of the numerical solution, the desingularized formulation of the BEM is used [3]. The considered coupled framework is illustrated by insightful examples.

[1] Wang, Q. X., and J. R. Blake. “Non-spherical bubble dynamics in a compressible liquid. Part 1. Travelling acoustic wave.” *Journal of Fluid Mechanics* 659 (2010): 191-224.
[2] Hughes, Thomas JR, John A. Cottrell, and Yuri Bazilevs. “Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement.” *Computer methods in applied mechanics and engineering* 194.39-41 (2005): 4135-4195.

[3] Klaseboer, Evert, Qiang Sun, and Derek YC Chan. "Non-singular boundary integral methods for fluid mechanics applications." *Journal of Fluid Mechanics* 696 (2012): 468-478.

Immersed isogeometric analysis with boundary-conformal quadrature for large deformation thermo-elasticity

Elbadry, Yusuf T. *(Cyber-Physical Simulation Group & Graduate School of Computational Engineering, Technical University of Darmstadt)*
Antolin, Pablo *(Institute of Mathematics, École Polytechnique Fédérale de Lausanne 1015 Lausanne, Switzerland)*
Weeger, Oliver *(Cyber-Physical Simulation Group & Graduate School of Computational Engineering, Technical University of Darmstadt)*

16:20

Numerical simulation of complex geometries can be costly and time consuming, in particular due to the long process of preparing the geometry for meshing and the meshing process itself [1]. Several methods were proposed to overcome this issue, such as the extended finite element, meshless, Fourier transform and immersed boundary methods. Immersed boundary methods rely on embedding the physical domain into a Cartesian grid of finite elements and resolving the geometry only by adaptive numerical integration schemes. For instance, the isogeometric finite cell method (FCM) exploits the accuracy of higher-order, smooth B-Spline basis functions for the discretization and employs an octree scheme in order to refine the quadrature rule in trimmed elements. FCM has been applied successfully to various problems in solid mechanics, including linear and nonlinear elasticity, elasto-plasticity, and thermo-elasticity [2]. However, FCM typically requires several levels of refinement of the quadrature rule in order to deliver accurate results, which may lead to high computation times, especially for nonlinear and internal variable problems.

In this work, we adopt a novel algorithm for boundary-conformal quadrature based on a high-order reparameterization of trimmed elements [3] to solve elasticity problems using spline-based immersed isogeometric analysis (IGA) without the need for a body conformal finite element mesh. In particular, the Gauss points on trimmed elements are obtained by a NURBS reparameterization of the physical subdomains of the cut elements of the Cartesian grid. This ensures an accurate integration with a minimal number of quadrature points. The 2D plate with a hole problem is used as a main benchmark to compare the algorithm with conformal isogeometric analysis and the finite cell method. The results show a convergence behavior for the adopted boundary conformal immersed IGA close to the one of the conformal IGA, which demonstrates the accuracy and efficacy of the method. Moreover, the approach is extended towards thermo-elasticity and finite deformation nonlinear elasticity.

[1] T. Hughes, J. Cottrell, and Y. Bazilevs. Isogeometric analysis: CAD, finite elements, NURBS, exact geometry and mesh refinement. *Computer Methods in Applied Mechanics and Engineering*, 194:4135- 4195, 2005.
[2] Schillinger, D. and Ruess, M., 2015. The Finite Cell Method: A review in the context of higher-order structural analysis of CAD and image-based geometric models. *Archives of Computational Methods in Engineering*, 22(3), pp.391-455.
[3] Wei, X., Marussig, B., Antolin, P. and Buffa, A., 2021. Immersed boundary-conformal isogeometric method for linear elliptic problems. *Computational Mechanics*, 68(6), pp.1385-1405.

Neural network based coupling of CALPHAD and the FEM in thermo-chemo-mechanical calculations

Roth, Stephan *(TU Bergakademie Freiberg, Germany)* 16:40
Zienert, Tilo *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*

Modeling thermo-chemo-mechanical coupling is of increasing interest in the investigation of processes such as stress corrosion cracking, hydrogen embrittlement, etc. Phase-field models that capture, e.g., diffusion, degradation, and phase-transformations, require the formulation of the chemical energy as a contribution to a total potential to be minimized in a variational framework [1]. The chemical energy, as a function of composition and temperature, can be incorporated using the CALPHAD method, either by direct implementation of the CALPHAD model with known parameters from databases or by calling an external CALPHAD software such as Thermo-Calc. In finite element (FE) simulations, the latter approach neccessitates a coupling of FE software to CALPHAD software, since the state potential has to be calculated in each integration point of the model, for each solution increment. In order to avoid sequential calls of external CALPHAD-software, which would drastically increase the overall computation time, here a numerical approach based on neural networks (NN) is proposed. The idea is to train the neural network with CALPHAD data such that the NN represents the chemical energy in relatively wide ranges of composition and temperature. The trained NN can then be included as a Fortran code to the computational framework and provides the chemical energy as well as its derivatives without any external software. The latter is only required for providing the training and validation data needed to calibrate the NN. Here, we specifically make use of the free Python library ffnet [2]. The procedure is demonstrated and verified by the example of a simple Ag-Au-diffusion couple with well defined chemical energies. The comparison between a direct and the NN-based implementation is drawn, demonstrating the quality of the proposed approach. Finally, the applicability to more complex multi-component, multi-phase problems, see [3], is addressed.

[1] B. Svendsen, P. Shanthraj, and D. Raabe. Finite-deformation phase-field chemomechanics for multiphase, multicomponent solids. JMPS, 112:619-636, 2018.
[2] M. Wojciechowski. ffnet 0.8.3, `https://ffnet.sourceforge.net/`.
[3] A. Seupel, S. Roth, and B. Kiefer. Phase-field modeling of chemically reactive multicomponent/multi-phase systems. PAMM, 10.1002/pamm.202200154, 2022.

A FEM-PD coupling based on an Arlequin approach to impose boundary conditions in Peridynamics

Pernatii, Anna *(Otto-von-Guericke Universität Magdeburg, Germany)* 17:00
Gabbert, Ulrich *(Otto-von-Guericke Universität Magdeburg, Germany)*
Willberg, Christian *(German Aerospace Centre (DLR) Braunschweig, Germany)*
Hesse, Jan-Timo *(German Aerospace Centre (DLR) Braunschweig, Germany)*

The peridynamic approach (PD) is a continuous theory that is well suited for solving damage problems. Because of the non-local formulation, PD can predict the response of a material and fracture patterns with high probability in high dynamic processes. In PD, some parameters differ from the continuum formulation and have some deviation in discretized PD systems, such as a horizon. A material constant becomes a parameter dependent on the mesh

size.
A sticking point, which has to be considered, is that an incomplete horizon at the boundaries results in an unphysical variation of the material's stiffness in these regions. Material points at the boundaries do not have an entire non-local neighborhood, meaning the points have fewer bonds and are softer than points within the domain. This leads to the so-called surface effect. The difficulties in applying the classical local initial and boundary conditions happen because of the non-local character of the PD. To overcome this problem, several correction techniques have been developed. Nevertheless, a standard method to describe them is not available yet.
An alternative approach is the application of the earlier proposed FEM-PD coupling, which can be seen as a local-nonlocal coupling method. The damage-free zones are analyzed by the FEM as classical local theory, while the domain where the fracture is expected is modeled with the PD as a non-local theory. Consequently, the reduction of the computational effort as well as the imposing of the conventional local boundary conditions, is achieved. The coupling method is based on the Arlequin method - an energy-based procedure where the energy of a system is found as a weighted average of both systems. The mechanical compatibility in the overlapping zone of both domains is reached by implementing constraints with the help of the penalty method. In the paper at hand, the focus is on imposing BCs. The proposed method is applied to both static and dynamic applications. The accuracy and convergence behavior is evaluated by analyzing test examples.

Adaptive time integration for dynamic problems in the Theory of Porous Media using an EVI-formulation

Sunten, Julia Nicolina *(University of Duisburg-Essen, Germany)* 17:20
Schwarz, Alexander *(University of Duisburg-Essen, Germany)*
Bluhm, Joachim *(University of Duisburg-Essen, Germany)*
Schröder, Jörg *(University of Duisburg-Essen, Germany)*

In classical binary (Solid and Liquid) dynamic Theory of Porous Media (TPM) formulations, two dependent factors influence the numerical efficiency: The number of unknown quantities and the choice of the time integration scheme. Following the approach of Diebels and Ehlers in [1], the disadvantage of ten scalar unknowns ($U_{DE} = \{u_S, v_S, w_{LS}, P\}$, Solid displacement, Solid velocity, difference velocity, pore pressure) is compensated by the full range of possible time integration schemes as the relations $u'_S = v_S$ and $u''_S = v'_S$ can be treated by any implicit time integration method. On the other hand, the approach of Breuer in [2] only requires seven scalar unknown quantities ($U_B = \{u_S, w_{LS}, P\}$), but depends on the existence of a time integration method which is able to determine the second material time derivative of the Solid displacement. To overcome this dependency drawback Chen et al, see [3], presented the idea of an EVI-formulation (Embedded Velocity Integration), where the unknowns are $U_{EVI} = \{v_S, w_{LS}, P\}$. The Solid displacement is now determined as the temporal integration and the acceleration as the temporal derivative of the Solid velocity. This contribution presents the idea of [3] and combines it with an adaptive explicit singly diagonally implicit Runge-Kutta scheme, see [4], which was already used for TPM problems in [5]. Thereby a maximum of numerical

efficiency for dynamic geomechanical problems is gained and the method is compared to the classical approach of [1].

[1] S. Diebels and W. Ehlers. Dynamic analysis of a fully saturated porous medium accounting for geometrical and material non-linearities. International Journal for Numerical Methods in Engineering, 39:81-97, 1996.
[2] S. Breuer. Dynamic response of a fluid -saturated elastic porous solid. Archive of Mechanics, 49:791-804, 1997.
[3] Z. Chen, H. Steeb and S. Diebels. A EVI-space-time Galerkin method for dynamics at finite deformation in porous media. Computational Mechanics, 43:585-601, 2009.
[4] J.R. Dormand and P.J. Prince. A family of embedded Runge-Kutta formulae. Journal of Computational and Applied Mathematics, 6:19-26, 1980.
[5] P. Ellsiepen. Zeit-und ortsadaptive Verfahren angewandt auf Mehrphasenprobleme poröser Medien. PhD-Thesis, Universität Stuttgart, 1999.

An Efficient Newton-multigrid FEM Solver for Multifield Nonlinear Problems Applied to Thixo-viscoplastic Flows

Begum, Naheed *(TU Dortmund University, Germany)* 17:40
Ouazzi, Abderrahim *(TU Dortmund University, Germany)*
Turek, Stefan *(TU Dortmund University, Germany)*

In this talk, we shall be concerned with efficient Newton-multigrid FEM solver for multifield nonlinear flow problems. In our approach, for efficient FEM solver, we reveil and advantageously use the delicate symbiosis aspects of the problem settings for FEM approximations, and the algorithmic tools to obtain the approximated numerical solutions. We concretize our ideas on thixo-viscoplastic flow problems. It is a two-field coupled nonlinear problem. And beside the integrated nonlinearity within momentum equation and microstructure equation, thixo-viscoplastic problems induce a nonlinear two way coupling. As far as FEM numerical solutions is concerned, we set the problem in a suitable variational form and proceed with the corresponding analysis of wellposdness. Indeed, our wellposedness study is
not an intellectual exercise, rather it is the foundation for the approximate problem as well as for the development of the efficient solver. Here, we provide the wellposedness results for thixo-viscoplastic problem in FEM settings and the
error analysis of the approximate problem. We proceed in the same context to develop a monolithic Newton-multigrid TVP solver. We handle the nonlinearity of the problem in black box framework using an adaptive combined discrete Newton's and monolithic geometric multigrid solver. The linear systems are solved in a block Gauss-Seidel way, where the construction of the blocks is based on incompressibility constraint. Furthermore, with our choice of discontinuous linear pressure, we efficiently handle the problem coupling locally. And to maintain the solver efficiency with the fact of noncoupling of pressure and microstructure, we collocate the microstructure with the velocity in the quadratic interpolation. We provide a bunch of numerical simulations to support the accuracy, robustness, and efficiency of our approach. The material of this talk is based on our below recent work.

S07-11: Coupled problems

Date: June 2, 2023 16:00-18:00
Room: CHE/183

A mixed least-squares finite element method for a geometrically nonlinear TPM formulation

Schwarz, Alexander *(University of Duisburg-Essen, Germany)* 16:00
Schwarz, Carina *(University of Duisburg-Essen, Germany)*
Bluhm, Joachim *(University of Duisburg-Essen, Germany)*
Schröder, Jörg *(University of Duisburg-Essen, Germany)*

In the present work, a mixed least-squares finite element method (LSFEM) is used, which is applied on the partial differential equations arising from the Theory of Porous Media (TPM), see e.g. [1, 2, 3]. Since the LSFEM is not limited to the LBB condition, the method has some theoretical advantages over the well-known (mixed) Galerkin method, see [4]. In particular, the LSFEM leads to positive definite and symmetric system matrices, even for differential equations with non-self-adjoint operators, see e.g. [5]. In detail, we study an incompressible binary model with solid and liquid phases. The modeling of saturated porous structures serves as the basis for the presented approach. The resulting finite element is a four-field formulation in terms of solid displacements, fluid pressure, mixture stresses, and a new variable associated with the pressure gradient. Vector-valued Raviart-Thomas and conventional Lagrangian functions are used to achieve a conforming discretization of the unknowns in the spaces H(div) and H1. The applicability of the LSFEM approach is demonstrated with numerical examples for fluid-saturated porous structures, which consider incompressible, geometrically nonlinear elastic material behavior.

[1] R.M. Bowen. Incompressible porous media models by use of the theory of mixtures. International Journal of Engineering Sciences 18:1129-1148, 1980.
[2] R.M. Bowen. Compressible porous media models by use of the theory of mixtures. International Journal of Engineering Sciences 20:697-735, 1982.
[3] W. Ehlers, J. Bluhm (Eds.): Porous media: Theory, experiments and numerical applications. Springer, 2002.
[4] P.B. Bochev and M.D. Gunzburger. Least-Squares Finite Element Methods. Springer-Verlag, New York, 1st edition, 2009.
[5] Z. Cai, B. Lee, and P. Wang. Least-squares methods for incompressible Newtonian fluid flow: Linear stationary problems, SIAM J. Numer. Anal., 42(2):843-859, 2004.

A coupled finite element TPM formulation for the modeling of freezing processes using a discontinuous approximation for the volume fraction ice

Koßler, Marvin *(University of Duisburg-Essen, Germany)* 16:20
Schwarz, Alexander *(University of Duisburg-Essen, Germany)*
Bluhm, Joachim *(University of Duisburg-Essen, Germany)*
Schröder, Jörg *(University of Duisburg-Essen, Germany)*

In this work, a multiphase approach for the modeling of freezing processes in the context of a coupled finite element formulation using the Theory of Porous Media (TPM) is presented, see also [1]. Here, the focus is on improving numerical stability within a standard Galerkin procedure regarding the volume fraction ice, which is highly sensitive to discontinuities within the domain. To solve this problem, a discontinuous approximation for the volume fraction ice is utilized while the remaining degrees of freedom are still approximated continuously. This leads to the corresponding degrees of freedom being solved independently for each element as the nodes of the elements are not tied to other elements. In order to underline the optimization effect, numerical examples are evaluated. These examples feature results using both the continuous as well as discontinuous approximation for the volume fraction ice and are set in contrast to each other. In a further step, the implementation of the discontinuous approximation enables the application of static condensation, leading to a reduced computing time.

References:

[1] A. Schwarz, J. Bluhm und J. Schröder. "Modeling of freezing processes of ice floes within the framework of the TPM". In: Acta Mechanica 231 (2020), S. 3099-3121. https://doi.org/10.1007/s00707-020-02686-8.

Numerical simulation of miscible multiphase flow and fluid-fluid interaction in deformable porous media

Peters, Sven *(RWTH Aachen University, Germany)* 16:40
Heider, Yousef *(RWTH Aachen University, Germany)*
Markert, Bernd *(RWTH Aachen University, Germany)*

The focus of the underlying research work is on the macroscopic modeling of unstable multiphase fluid flow in deformable porous media, where a lower viscous fluid is displaced by a more viscous fluid. This process leads to the formation of channel-like structures, called viscous fingering. The instability effect is involved in a wide range of different fields in engineering. Some of the most common applications include carbon sequestration to store carbon dioxide (CO2) in underground reservoirs, contaminant transport in geostructures, in industrial processes, such as filtration, catalytic reactions, and in the operation of polymer electrolyte membrane fuel cells with multiphase flow in the gas diffusion layers, see, e.g, [1]. In this work, ideal miscible water-glycerin fluids are considered. It is assumed that the interacting fluids in the deformable porous media are incompressible. In addition, an isotropic dispersion-diffusion law is applied to capture the fluid-fluid interactions [2]. The presence of deformable porous material adds additional effects to the problem of the multiphase flow in porous media. The stresses in the porous solid matrix lead to changes in the porosity and influence the flow velocity of the fluids [3]. To couple the deformable porous media with the multiphase flow, a macroscopic approach is used that relies on the Theory of Porous Media

(TPM). For the porous solid matrix, a linear elastic material model within small strains assumption is applied. The influence of the deformation-dependent porosity to the instability is studied for 2D simulations, such as a multilayered geometry with different elastic parameters. The presented coupled nonlinear system of differential equations is simulated with the finite element method (FEM). Furthermore, a stabilization technique based on the Pressure-Laplacian-Projection Method is used.

[2] Chaaban, M., Heider, Y., and Markert, B (2022): A multiscale LBM-TPM-PFM approach for modeling of multiphase fluid flow in fractured porous media. *International Journal for Numerical and Analytical Methods in Geomechanics*, 46: 2698- 2724.
[2] Nijjer, J., Hewitt, D., and Neufeld, J. (2018): The dynamics of miscible viscous fingering from onset to shutdown. *Journal of Fluid Mechanics*, 837, 520-545. https://doi.org/10.1017/jfm.2017.829
[3] Markert B. (2007): A constitutive approach to 3-d nonlinear fluid flow through finite deformable porous continua; With application to a high-porosity polyurethane foam. *Transp Porous Med*.70:427-450. https://doi.org/10.1007/s11242-0079107-6

A Mixed Hu-Washizu-type Variational Formulation for Second-Gradient Poroelasticity

Khurshid, Hamza *(University of Stuttgart, Germany)*
Polukhov, Elten *(University of Stuttgart, Germany)*
Keip, Marc-André *(University of Stuttgart, Germany)*

17:00

The ubiquity of porous materials in nature makes them an important class of materials in various engineering fields. Understanding and predicting the behavior of such materials under different boundary and loading conditions can help us leverage them for a variety of applications. Computational models can help us to achieve this goal. First-gradient models of poroelasticity, despite their utility, fail to predict the boundary layer effects that arise near the drainage boundaries in the standard consolidation problem. Second-gradient theories can help us to get a more accurate picture of the behavior of porous materials near the boundaries. Sciarra et al. [1] have presented a second-gradient Biot-like theory of poromechanics that accurately predicts the boundary layer effects that arise near the drainage boundaries of porous material for the standard one-dimensional consolidation problem. Miehe et al. [2] have presented a variational formulation and finite-element implementation of two-field-minimization problem for the first-gradient theory in poroelasticity. The two fields under consideration are the displacement and fluid-flux fields. In the present contribution, we present a mixed Hu-Washizu-type variational saddle point formulation for poroelasticity based on the work [1]. In addition to the displacement and fluid mass content, we also consider their gradients in the free energy function. We solve the problem with the finite element method using C^0-continuous Lagrange functions for all primary fields. Additionally, we also present an alternative finite-element implementation where the fluid mass flux is interpolated using Raviart-Thomas shape functions. Finally, we present numerical examples depicting the second-gradient effects in porous materials.

[1] G. Sciarra, F. Dell'Isola and O. Coussy, Second gradient poromechanics. International Journal of Solids
and Structures (2008), 6607-6629.

[2] C. Miehe, S. Mauthe and S. Teichtmeister, Minimization principles for the coupled problem of Darcy-Biot type
fluid transport. Journal of the Mechanics and Physics of Solids 82 (2015), 186-217.
[3] S. Teichtmeister, S. Mauthe and C. Miehe, Aspects of finite element formulations for the coupled problem of poroelasticity based on a canonical minimization principle Computational Mechanics, 64 (2019), 685-716.

Analytical solution of dielectric two-domain problem and implications for interface conditions and crack tip loading

Behlen, Lennart *(University of Kassel, Germany)* 17:20
Wallenta, Daniel *(University of Kassel, Germany)*
Ricoeur, Andreas *(University of Kassel, Germany)*

Aside from mechanical stresses, dielectric ceramics may be subjected to electric fields for the purpose of multifunctional applications, especially with regard to piezoelectrics. Consequently, fracture analysis of these brittle materials is particularly concerned with the impact of an electric field on the loading situation at crack tips, and thus with appropriate electric and mechanical boundary conditions at the crack faces.

Accounting for the electric permeability of a mechanically distorted crack without solving coupled two-domain problems with electric interface conditions of bulk material and crack medium, the so-called capacitor analogy treats each two opposite points on the opened upper and lower crack faces as one-dimensional plate capacitor, enabling the employment of approximated surface charge densities on the boundaries as functions of the unknown voltage and distance between both points. Accommodating the electrostatic energy of the crack medium, the model was later complemented by Coulombic tractions acting on the crack faces, which emanate from the true Maxwell surface tractions under suitable simplifications. While the quality of the capacitor analogy has been investigated numerically for inclined electric loads with regard to the approximated surface charges, a likewise assessment of the Coulombic tractions is still pending, in particular considering curvature of crack faces prevailing under load.

In this work, the analytic solution of an elliptic cavity in an infinite dielectric is taken as basis, where a Griffith crack is obtained by letting the semi-minor axis tend towards zero. Both surface charges and tractions are examined with respect to their dependency on oblique remote electric fields as well as permittivities of bulk material and cavity. Moreover, the intensity factors prevailing at a mechanically opened crack of elliptic shape are determined with the aid of crack weight functions and finally compared to the values resulting from the capacitor analogy. As turns out, the surface charges represent an excellent substitute for the exact electric boundary conditions within a broad range of parameters, whereas large errors of the Coulombic tractions near the crack tip lead to a significantly underestimated mode I stress intensity factor.

Nonclassical Potential for the Two States Analysis

Göttlicher, Manfred *(University of Applied Sciences Erfurt, Germany)* 17:40

The nonclassical approach exchanges the role of variables. The variation refers not to physical variables directly. Instead, the distribution of the behavior on solid and liquid states is

subjected to variation. On the other side displacements, velocities and stresses are said to be constant according to the related mere solid or mere liquid single state analysis [1],[2].

In the classical potential [3] the elastic stiffness is present completely even if the solid specific weight is zero. The advantage of the nonclassical potential is the correlation between partial specific weight and stiffness. By this the permitted solution space is extended significantly.

At least for the standard application to the infinite high tube [3] an instant non continuous change of load results in an instant non continuous change of state. In the boundary load driven analysis, the distribution on static elastic solid and steady state incompressible viscous liquid parts follows the distribution of the boundary load that is restricted to the range between mere solid and mere liquid load.

The nonclassical potential bases on an area integral of the normal part of the elastic energy of the hybrid material. Two boundary integrals refer to the potential of the boundary load of the elastic part which results from the total boundary load reduced by the boundary load on the liquid part. Area load and wall interaction have no impact on the distribution on the two states.

Stresses are superimposed from both states according to the obtained distribution function in a secondary analysis. Displacements result from the contribution of the solid state. Velocities and liquid pressure result from the contribution of liquid state. Negative contributions are not permitted. Since the solid state at the beginning of time and the liquid state at the end of time are fixed, the distribution function can be seen as the influence of time.

[1] Reckling, K.A., Gummert, P.: Mechanik, 3rd ed., Springer: Berlin, 2014.

[2] Zienkiewicz, O.C., Taylor, R.L., et. al.: Finite Element Method, Vol. 1 to 3, 7th ed., Butterworth-Heinemann: Oxford, 2013.

[3] Göttlicher, M. Hybrid Analysis for Continua with Solid and Liquid Properties in Infinite High Tubes, Coupled Problems 2019, E. Oñate, M. Papadrakakis and B. Schrefler (Eds.), Barcelona, 2019.

S08: Multiscales and homogenization

Organizer(s): **Keip, Marc-André** *(U Stuttgart)*
Hesch, Christian *(U Siegen)*

S08-01: Multiscales and homogenization

Date: May 30, 2023 13:30-16:10
Room: HSZ/H03

Micromorphic multi-scale simulation of the elastic-plastic behavior of foams

Malik, Alexander *(TU Bergakademie Freiberg, Germany)* 13:30
Hütter, Geralf *(TU Bergakademie Freiberg, Germany; BTU Cottbus - Senftenberg, Germany)*
Abendroth, Martin *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*

Foam materials have mesostructures with characteristic cell sizes up to the millimeter regime, so that even engineering structures may not seldom consist of a few layers of foam cells. The macroscopic mechanical properties appear to be dependent on the structural size. Reason for such size effects is, that disturbed layers are formed near surfaces or in regions of strong gradients. The classical homogenization theory of Hill, which is based on the assumption of locally negligible gradients of deformations over a single cell, is not able to capture described effects.

Due to this, a micromorphic homogenization framework is used in the present contribution within a Direct-FE^2 implementation to simulate such size effects in the elastic-plastic behavior of foam structures. Different subclasses of the micromorphic theory are used as well as an unrestricted micromorphic theory. The results are benchmarked for simple loading cases like pure bending, for which even analytical solutions do exist partly, before the behavior of more complex structures is simulated. Finally, the results are compared with (more expensive) direct numerical simulations (DNS) of the fully resolved mesostructure of foam structures.

Modeling large-scale acoustic meta-structures through the reduced relaxed micromorphic model

Rizzi, Gianluca *(TU Dortmund, Germany)* 14:10
Voss, Jendrik *(TU Dortmund, Germany)*
Hermann, Svenja *(TU Dortmund, Germany)*
Collet, Manuel *(École Centrale de Lyon, France)*
Neff, Patrizio *(Universität Duisburg-Essen, Germany)*
Madeo, Angela *(TU Dortmund, Germany)*

In the framework of elastic waves propagation, it is nowadays clear that only non-local or higher-order models are able to properly describe micromechanical effects in solids with microstructures or heterogeneities.

Two common examples of such micromechanical effects are the presence of *band gaps*, which are frequency ranges for which the propagation of waves is inhibited, and *size effects*, which

describes the change of the response of a structure while changing the ratio between its dimensions and the size of the unit cell that characterizes it.

In order to reproduce these effects with a continuous material, the reduced relaxed micromorphic model is here proposed [1,2].

After the reduced relaxed micromorphic model's parameters are fitted on the dispersion curves of the material of interest (obtained via a Bloch-Floquet analysis), its reliability is assessed through the comparison of the response of finite-size structures for several loads conditions, which are differing in terms of frequencies and directions of propagation [2,3], and with real experiments on finite-size samples [3].

The mechanical behaviour of different unit cells is explored with the intent of optimize the position and the extent of band-gaps while tuning the magnitude of size effects, and connections between some of the geometrical and material features of the unit cell and the parameters of the reduced relaxed micromorphic model are established.

[1] Rizzi, G., Collet, M., Demore, F., Eidel, B., Neff, P. & Madeo, A. Exploring metamaterials' structures through the relaxed micromorphic model: switching an acoustic screen into an acoustic absorber. Frontiers In Materials. 7 pp. 589701 (2021)
[2] Rizzi, G., D'Agostino, M., Neff, P. & Madeo, A. Boundary and interface conditions in the relaxed micromorphic model: exploring finite-size metastructures for elastic wave control. Mathematics And Mechanics Of Solids. 27, 1053-1068 (2022)
[3] Demore, F., Rizzi, G., Collet, M., Neff, P. & Madeo, A. Unfolding engineering metamaterials design: relaxed micromorphic modeling of large-scale acoustic meta-structures. Journal Of The Mechanics And Physics Of Solids. 168 pp. 104995 (2022)
[4] Rizzi, G., Neff, P. & Madeo, A. Metamaterial shields for inner protection and outer tuning through a relaxed micromorphic approach. Philosophical Transactions Of The Royal Society A. 380, 20210400 (2022)

Parameter Identification in the Relaxed Micromorphic Model

Sarhil, Mohammad *(Institut für Mechanik, Universität Duisburg-Essen, Germany)*
Scheunemann, Lisa *(Lehrstuhl für Technische Mechanik, RPTU Kaiserslautern-Landau, Germany)*
Schröder, Jörg *(Institut für Mechanik, Universität Duisburg-Essen, Germany)*
Neff, Patrizio *(Lehrstuhl für Nichtlineare Analysis und Modellierung, Universität Duisburg-Essen, Germany)*

14:30

The use of enriched continua is a suitable choice for the modeling of microstructured materials, such as metamaterials, for which the scale-separation criterion does not hold. The relaxed micromorphic model [1] has demonstrated many advantages over other higher-order continua. The most notable advantage is using fewer material parameters and the drastically simplified strain energy compared to the classical micromorphic theory. The relaxed micromorphic model operates between two bounds which allows us to define two well-separated scales; the micro and macro elasticity tensors. Moreover, it controls the size-effect phenomena via one length scale parameter with keeping the other parameters scale-independent. The strain energy function in the relaxed micromorphic model employs the Curl of

a nonsymmetric second-order micro-distortion field and therefore H(Curl)-conforming FEM implementation is necessary [2].

In our talk, we present our recent findings in identifying the material parameters and boundary conditions in the relaxed micromorphic model, [3].

[1] P. Neff, I.D. Ghiba, A. Madeo, L. Placidi and G. Rosi. A unifying perspective: the relaxed linear micromorphic continuum. Continuum Mechanics and Thermodynamics 26,639-681(2014).
[2] J. Schröder, M. Sarhil, L. Scheunemann and P. Neff. Lagrange and H(curl,B) based Finite Element formulations for the relaxed micromorphic model, Computational Mechanics 70, pages 1309-1333 (2022).
[3] M. Sarhil, L. Scheunemann, J. Schröder, P. Neff. Size-effects of metamaterial beams subjected to pure bending: on boundary conditions and parameter identification in the relaxed micromorphic model. https://arxiv.org/abs/2210.17117(2022).

Size effects in numerical homogenization of polycrystalline silicon

Weber, Martin *(Otto-von-Guericke-Universität Magdeburg, Germany)*
Aßmus, Marcus *(Otto-von-Guericke-Universität Magdeburg, Germany)*
Glüge, Rainer *(Otto-von-Guericke-Universität Magdeburg, Germany)*
von Zabiensky, Max *(Otto-von-Guericke-Universität Magdeburg, Germany)*
Altenbach, Holm *(Otto-von-Guericke-Universität Magdeburg, Germany)*

14:50

A current topic in the photovoltaic industry is the analysis and evaluation of possible structural and material properties. This requires the effective material characteristics of polycrystalline silicon, which is an important component for the functional performance of the photovoltaic modules in use. Since this assessment is associated with high costs, it is to be carried out already in the product development process. Due to very thin silicon layers, the effect of the layer thickness on the effective material characteristics has to be investigated (see [1,2]). In this work, a procedure to determine these characteristic values is listed to investigate the size effect on different film thicknesses of this material. With the knowledge of the properties of the silicon single crystal with its cubic symmetry on the micro level, a homogenization of the properties to the macro level can be done. The polycrystal structure with a cubic sample geometry forms the macro level. This structure is now cut into thinning layers for investigation. The open-source software Neper is used to create the crystal structure and the interconnectivity for this purpose. With the help of Matlab, this information is passed on to the finite element program Abaqus, where the results are evaluated after an elastic calculation using Python. The focus is on the expected change in material properties as a function of the layer thickness. Finally, the method according to [3] is also used to investigate the change in material symmetry.

References:

[1] Aßmus, M., Glüge, R. and Altenbach, H., On the analytical estimation for isotropic approximation of elastic properties applied to polycrystalline cubic silicon used at solar cells,Technische Mechanik, 40(2):120-133, 2020
[2] Glüge, R., Altenbach, H., Mahmood, N. and Beiner, M., On the difference between the tensile stiffness of bulk and slice samples of microstructured materials, Applied Composite Materials, 27(6):969-988, 2020

[3] Weber, M., Glüge, R. and Bertram, A., Distance of a stiffness tetrad to the symmetry classes of linear elasticity, International Journal of Solids and Structures, 156-157:281-293, 2019

Unfolding engineering metamaterials design: relaxed micromorphic modeling of large-scale acoustic meta-structures.

Erel-Demore, Felix *(Technical University of Dortmund, Germany)*
Rizzi, Gianluca *(Technical University of Dortmund, Germany)*
Collet, Manuel *(Ecole Centrale de Lyon, France)*
Neff, Patrizio *(University of Duisburg-Essen, Germany)*
Madeo, Angela *(Technical University of Dortmund, Germany)*

15:10

We present a unit cell showing a band-gap (i.e. able to inhibit wave propagation) in the lower acoustic domain. The corresponding metamaterial is made up of a periodic arrangement of one unit cell. We rigorously show that the relaxed micromorphic model can be used for metamaterials' design at large scales as soon as sufficiently large specimens are considered. We manufacture the metamaterial via metal etching procedures applied to a titanium plate so as to show that its production for realistic applications is viable. Experimental tests are also carried out confirming that the metamaterials' response is in good agreement, with some additional recalibration procedure, with the theoretical design. In order to show that our micromorphic model opens unprecedented possibilities in metastructural design, we conceive a finite-size structure that is able to focus elastic energy in a confined region, thus enabling its possible subsequent use for optimizing complex structures. Indeed, thanks to the introduction of a well-posed set of micromorphic boundary conditions, we can combine different metamaterials and classical Cauchy materials in such a way that the elastic energy produced by a source of vibrations is focused in specific collection points. The design of this structure would have not been otherwise possible (via e.g., direct simulations), due to the large dimensions of the metastructure, couting hundreds of unit cells. Finally, we present and justify the ability of the homogenised relaxed micromorphic model to predict the response of microstructured structured independently of unit cell's chosen geometry.

Comparison of different homogenization approaches for the inelastic behavior of porous structures

Abendroth, Martin *(TU Bergakademie Freiberg, Germany)*
Malik, Alexander *(TU Bergakademie Freiberg, Germany)*
Lange, Nils *(TU Bergakademie Freiberg, Germany)*
Hütter, Geralf *(TU Bergakademie Freiberg, Germany)*
Kiefer, Björn *(TU Bergakademie Freiberg, Germany)*

15:30

The direct numerical simulation (DNS) of highly porous structures is computationally very expensive, whereas homogenization approaches are considered to reduce computational costs. This contribution compares different homogenization approaches for porous structures. First approach is a constitutive analytical model based on a model for granular media of Ehlers. The second approach is a FE^2 homogenization developed by N. Lange. Third, a hybrid approach using neural networks within a constitutive framework to model the inelastic deformation behavior of porous structures. Named approaches are compared with respect to their accuracy, efficiency, generality, and necessary effort to generate them.

S08-02: Multiscales and homogenization

Date: May 31, 2023 08:30-09:30
Room: HSZ/H03

Modeling the material behavior of heterogeneous materials considering a two-scale FE-FFT-based simulation framework

Schmidt, Annika *(RWTH Aachen University, Germany)* 08:30
Gierden, Christian *(RWTH Aachen University, Germany)*
Waimann, Johanna *(RWTH Aachen University, Germany)*
Reese, Stefanie *(RWTH Aachen University, Germany)*

In various engineering applications, components subjected to high mechanical or multi-physical loads such as thermal, thermo-mechanical or electro-thermal loads are predominantly made of metals or composites. These materials are characterized by polycrystalline or multiphase microstructures which determine the overall material response. However, since the microscopic material behavior is directly related to the distribution, size and morphology of the individual grains or phase-constituents, precise predictions of the macroscopic material response require simulations of the microstructural behavior. Hence, this work considers a two-scale finite element (FE) and fast Fourier transform (FFT)-based simulation framework [1, 2], which is an efficient alternative to the classical FE^2 method for the simulation of periodic unit cells [3]. Assuming scale separation, the macroscopic and microscopic boundary value problems are first solved individually and subsequently linked by performing a scale transition in terms of averaging the macroscopic quantities over the corresponding local fields. While the macroscopic solution is computed by means of the finite element method, the microscopic boundary value problem, which is embedded as a periodic unit cell in each macroscopic integration point, is solved using a fast Fourier transform based simulation method. In general, these microscopic simulations allow to model grain-scale phenomena such as martensitic phase transformation or plastic deformation caused by dislocation glide which can be observed in polycrystalline materials. In order to demonstrate the applicability of the model, several numerical examples are given.

[1] J. Spahn, H. Andrä, M. Kabel, and R. Müller. A multiscale approach for modeling progressive damage of composite materials using fast Fourier transforms. Computer Methods in Applied Mechanics and Engineering, 268, 871-883, 2014
[2] J. Kochmann, S. Wulfinghoff, S. Reese, J. R. Mianroodi, and B. Svendsen. Two-scale FE-FFT- and phase-field-based computational modeling of bulk microstructural evolution and macroscopic material behavior. Computer Methods in Applied Mechanics and Engineering, 305, 89-110, 2016
[3] C. Gierden, J. Kochmann, J. Waimann, B. Svendsen and S. Reese. A review of FE-FFT-based two-scale methods for computational modeling of microstructure evolution and macroscopic material behavior. Archives of Computational Methods in Engineering, 29(6), 4115-4135, 2022.

An iterative multi-step solver for linear systems arising in the context of periodic phase-field problems

Krischok, Andreas *(University of Stuttgart, Germany)*
Yaraguntappa, Basavesh *(University of Stuttgart, Germany)*
Keip, Marc-André *(University of Stuttgart, Germany)*

08:50

We present a strategy for building a solver based on an analytical inversion of a matrix equation that arises from discretizing a strong form using a Fourier spectral method. The solver is constructed such that it resembles an iterative solver that only uses fast Fourier transforms for the necessary matrix-vector multiplications. In contrast to standardized solvers, the method represents a multi-step algorithm that, due to accessing previous iterations, is able to provide an attractive convergence speed. The approach is presented in the context of higher-order gradient flow problems in periodic unit cells and compared to standardized solvers such as the preconditioned conjugate gradient solver.

The talk discusses how the proposed method can be incorporated into phase-field methods that aim to optimize the compliance of periodic lattice structures under a given macroscopic load. Regarding the benefits of the method, an emphasis is given with respect to the competition between storage, speed, preconditioning and parallelization. We further discuss if and how the method can be used in the context of other linear systems that arise in the context of elastic composites and homogenization problems.

Composite Boxels with imperfect Interfaces (ComBI) with FFT-based solvers

Keshav, Sanath *(SC Simtech, Data Analytics in Engineering University of Stuttgart, Germany)*
Fritzen, Felix *(SC Simtech, Data Analytics in Engineering University of Stuttgart, Germany)*
Kabel, Matthias *(Department Flow and Material Simulation, Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM Kaiserslautern, Germany)*

09:10

Cohesive zones were first introduced to simulate the production of cracks caused by interfacial damage. However, the term is often used in a broader sense to refer to imperfect interfaces governed by constitutive traction separation laws. In unstructured finite element simulations, cohesive zones are discretized by specific interface-conforming cohesive elements. The discretization of FFT-based methods is generally non-conforming to the interfaces; hence the classical interface cohesive elements cannot be employed. In this work, we propose a framework that is a generalization of composite boxels [Keshav, S. Fritzen, F. Kabel, M. 2022, Kabel, M et al. 2015] for interfacial damage modeling in FFT-based solvers. The special focus is on gathering the interface metadata from images using a novel image-based algorithm. An efficient implementation with a particular emphasis on numerical robustness is proposed. Numerical examples along with traction and stress field statistics comparing the proposed framework with unstructured finite element simulations are presented.

S08-03: Multiscales and homogenization

Date: May 31, 2023 08:30-09:30
Room: HSZ/403

A phase-field approach for optimizing unit cells for structures with anisotropic properties

Yaraguntappa, Basavesh *(University of Stuttgart, Germany)* 08:30
Krischok, Andreas *(University of Stuttgart, Germany)*
Keip, Marc-André *(University of Stuttgart, Germany)*

Inspired by lattice structures that can be observed in nature, periodic unit cells and their mechanical properties have caused an ever increasing interest in recent years due to the growing performance of additive manufacturing meth-
ods. In order to incorporate cells with optimal properties into printed high-performance structures and devices that can respond to given stress-strain states due to macroscopic boundary conditions in an optimal manner, one has to pro-
vide anisotropic properties that can respond to individual loads in an optimal manner. We discuss the performance of a phase-field approach for optimizing periodic micro-structures based on triply periodic minimal surface problems (TPMS) to obtain unit cells with optimal homogenized stiffness response in the direction of the maximal principal stress direction. We show that different TPMS-types exhibit fundamental differences in the way they can respond to uni-axial or shear-dominated loads. An essential aspect in optimizing cells is, on the one hand, to maximize the compliance with external loads and, on the other hand, to limit the danger of failure due to local buckling which is achieved by preserving the connectivity of the cell grid. Further aspects that are discussed include numerical strategies to handle such high-resolution optimization problems in an efficient manner as well as strategies to verify the gain of the homogenized stiffness experimentally.

Coarse-grained phase-field crystal modeling of elasticity and plasticity

Salvalaglio, Marco *(TU Dresden, Germany)* 08:50

Comprehensive investigations of crystalline systems often require methods bridging atomistic and continuum scales. In this context, coarse-grained mesoscale approaches are of particular interest as they allow the examination of large systems and time scales while retaining some microscopic details. The so-called phase-field crystal (PFC) model conveniently describes crystals at relatively large (diffusive) time scales through a continuous periodic field corresponding to the atomic density. In the amplitude expansion of the PFC model (APFC), a coarse-grained description of this density is obtained by focusing on its complex amplitudes and, in turn, on their dynamics. These amplitudes vary on length scales larger than the atomic spacing but still retain details of the crystal lattice. In this contribution, the basics of the APFC model are first introduced. Numerical simulations based on the APFC model and the Finite Element Method are shown to reproduce interfaces among phases and defects structures efficiently, retaining details of the underlying crystal structure. The derivation of continuous deformation fields from the complex amplitudes, their connections with the elasticity theory, and the characterization of dislocations are then discussed [1,2]. The description of crystal

structures through amplitudes is shown to be a powerful framework connecting atomic-scale lattice deformations and continuum elasticity. Moreover, a microscopically-informed description of defects akin to dislocation dynamics approaches is obtained. Finally, representative applications are outlined, such as the self-consistent description of defect motion in binary systems with effects induced by Cottrell Atmospheres (solute segregation at defects) [3].

[1] J. Mech. Phys. Solids 137 103856, (2020)
[2] Model. Sim. Mater. Sci. Eng 30, 053001 (2022
[3] Phys. Rev. Lett. 126 185502 (2021)

Nonlinearly weighted homogenization of phase-field evolution laws involving spatial and temporal scale-separations

von Oertzen, Vincent *(TU Bergakademie Freiberg, Germany)*
Kiefer, Bjoern *(TU Bergakademie Freiberg, Germany)*
09:10

The evolution of microstructures involving complex interface topologies has been heavily investigated by means of phase-field methods for many years due to their spatial regularization capabilities. Accordingly, several important contributions were made in this regard, so that there exists a wide spectrum of well-established frameworks applicable to various multi-physics problems on different physical scales, see [1] and the references therein. However, a general notion for consistently transferring one specific phase-field model between several spatial, and also temporal, scales has still not been fully developed. Current homogenization schemes typically rely on many additional assumptions that drastically restrict the space of microscopic solution fields. Moreover, evolution rates may also differ up to several orders of magnitude between different physical quantities, especially in the context of multi-physical problems. Despite this, resulting difficulties related to consistently bridging these temporal scales are typically left out of conventional homogenization considerations.

To address this issue, the concept of unequally and nonlinearly weighted averaging operators, as introduced in [2], is applied to an Allen-Cahn based dual-phase system in order to derive its effective driving force on the relevant scale. Accordingly, numerical solutions of the resulting spatially and temporally homogenized evolution laws are shown to match those from finite element simulations of microstructure formation in ZrO_2, see [3], thus validating the outlined homogenization procedure. Its theoretical embedding within the context of finite scale-separations is then additionally discussed, which involves implicit definitions for macroscopic gradients and homogenized time derivatives.

References:

[1] T. Q. Bui and X. Hu, 2021. *A review of phase-field models, fundamentals and their applications to composite laminates*, Eng. Fract. Mech. 248, 107705.
[2] V. von Oertzen and B. Kiefer, 2022. *Unequally and non-linearly weighted averaging operators as a general homogenization approach for phase-field modeling of phase transforming materials*, Shape Mem. Superelasticity 8, 425–437.
[3] M. K. Rajendran, M. Kuna and M. Budnitzki, 2020. *Undercooling versus stress induced martensitic phase transformation: The case of MgO – partially stabilized zirconia*, Comput. Mater. Sci. 8, 109460.

S08-04: Multiscales and homogenization

Date: May 31, 2023 14:00-16:00
Room: HSZ/H03

Scattering Transform in Microstructure Reconstruction

Reck, Paul *(Universität Augsburg, Germany)* 14:00

Microstructure characterization and reconstruction (MCR) is a key enabler of process-structure-property linkages, a central topic in materials engineering [1]. Much progress has been made in MCR in the last years, however, in absence of a flexible software platform it is difficult to use ideas from other researchers and to develop them further. To address this issue, Seibert et al. [2] presented a flexible and extensible software MCRpy, which allows for descriptor based characterization and reconstruction of microstructures.
The choice of descriptor is crucial for the resulting characterization properties and is a current area of research. We exploit the extensibility of MCRpy and introduce a new type of descriptor, the Scattering Transform.
The Scattering Transform is a widely used tool in image processing, it's main advantage being translation invariance and Lipschitz continuity to the actions of diffeomorphisms [3]. The Lipschitz continuity could prove beneficial in the context of microstructure reconstruction in order to neglect small pertubations in the microstructure and in this talk we investigate the aforementioned potential.

Quellen:

[1] Reconstructing random heterogeneous media through differentiable optimization, `https://arxiv.org/abs/2103.09686`

[2] Microstructure Characterization and Reconstruction in Python: MCRpy, `https://arxiv.org/abs/2207.04652`

[3] Group Invariant Scattering, `https://arxiv.org/abs/1101.2286`

A microstructure-generation method for fiber composites accounting for fiber length and orientation distribution coupling

Mehta, Alok Ranjit *(Karlsruhe Institute of Technology, Germany)*
Schneider, Matti *(Karlsruhe Institute of Technology, Germany)* 14:20

Short Fiber Reinforced Polymers (SFRP) have gained their popularity due to their high strength to weight ratio, corrosion resistance and their manufacturability of the complex geometry in many applications. They are commonly produced by injection molding. The process inherently generates complex microstructure which might have layered constituents (skin-core-skin), different fiber lengths due to fiber breakage during the injection molding and different fiber orientations due to flow of the matrix material. It is evident that in SFRP, shorter fibers orient quickly whereas longer fibers re-orients more slowly during injection molding [1]. It can be inferred that there exists some kind of connection (coupling) between fiber lengths and fiber orientations. The Sequential Addition and Migration (SAM) algorithm [2] can be used to generate digital image of the microstructure which is then used in conjunction with computational homogenization methods to compute effective material properties. An extension of

the SAM Algorithm which originally assumes uncoupled behavior [3] for fiber length and orientation distributions is studied and presented. In reality there exists a connection between the two distributions. This work discusses coupled behavior using special case of Weibull fiber-length distribution. Also effects on mechanical properties for coupled and uncoupled approaches are compared and analyzed. Results are validated by showing a good agreement with multilayered industrial SFRP sample.

References

[1] J. Wang, J. F. O'Gara, and C. L. Tucker, "An objective model for slow orientation kinetics in concentrated fiber suspensions: Theory and rheological evidence," Journal of Rheology, vol. 52, pp. 1179-1200, 2008.

[2] M. Schneider, "The Sequential Addition and Migration method to generate representative volume elements for the homogenization of short fiber reinforced plastics," Computational Mechanics, vol. 59, pp. 247-263, 2017.

[3] A. Mehta and M. Schneider, "A sequential addition and migration method for generating microstructures of short fibers with prescribed length distribution," Comput. Mech., vol. 70, p. 829-851, oct 2022.

3D orientation map reconstruction using the 2-point correlation function in MCRpy

Safi, Ali Reza *(Helmholtz-Zentrum Hereon, Germany)* 14:40
Seibert, Paul *(TU Dresden)*
Kästner, Markus *(TU Dresden)*
Klusemann, Benjamin *(Helmholtz-Zentrum Hereon, Germany; Leuphana Universtiy Lüneburg)*

Microstructure Characterization and Reconstruction (MCR) is a key method used in materials science to produce 3D volume elements (VEs) from 2D imaging techniques such as electron-backscattered diffraction (EBSD). These VEs play a crucial role in crystal plasticity simulations, which examine the connection between a material's microstructure and its mechanical properties. The experimental methods for the extraction of 3D orientation maps suffer from being time and cost expensive which makes them unfeasible to perform high-throughput simulations and rises the demand for efficient MCR algorithms.

Descriptor-based MCR allows to extract microstructure descriptors from 2D techniques and optimizes the VE with respect to the descriptors of interest. Conventional MCR methods typically involve several steps, including the extraction of low-dimensional morphological descriptors like grain size distribution, anisotropy and polarity, as well as crystallographic descriptors like the orientation distribution function (ODF) and the misorientation distribution function (MDF) [1]. Although conventional descriptor-based MCR delivers satisfactory results for simple microstructures, it can be challenging to apply to materials produced through additive manufacturing or severe plastic deformation, which may have heterogeneous structures or extreme intragranular orientation gradients.

This work aims at solving these problems by formulating microstructure reconstruction for orientation maps as a flexible optimization problem based on generic, high-dimensional microstructure descriptors such as the 2-point orientation correlation function [2]. Building upon previous work for reconstructing multiphase microstructures [3], these descriptors are

formulated such that they are differentiable with respect to the microstructure parametrization and are implemented in the open-source software MCRpy. By performing reconstructions on various benchmark microstructures with unconventional features, the advantages of using MCRpy with the 2-point correlation function for reconstructing 3D orientation data will be illustrated. We thoroughly evaluate the reconstructions through detailed statistical analysis of morphological and crystallographic features.

References

[1] Groeber, Ghosh, Uchic, Dimiduk, A framework for automated analysis and simulation of 3D polycrystalline microstructures.: Part 1: Statistical characterization, Acta Materialia, 2008
[2] Paulson, Priddy, McDowell, Kalidindi, Reduced-order structure-property linkages for polycrystalline microstructures based on 2-point statistics, Acta Materialia, 2017
[3] Seibert, Raßloff, Ambati, Kästner, Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization, Acta Materialia, 2022

Statistical descriptors in structure-property linkages for inverse microstructure design

Raßloff, Alexander *(Technische Universität Dresden, Institute of Solid Mechanics, Germany)*
Seibert, Paul *(Technische Universität Dresden, Institute of Solid Mechanics, Germany)*
Kalina, Karl Alexander *(Technische Universität Dresden, Institute of Solid Mechanics, Germany)*
Kästner, Markus *(Technische Universität Dresden, Institute of Solid Mechanics, Germany; Technische Universität Dresden, Dresden Center for Computational Materials Science, Germany)*

15:00

In this contribution, we propose a general framework to examine structure-property linkages computationally using scarce data. Large databases of structure-property pairs are needed to derive profound correlations. Experiments alone, such as microscopy and mechanical tensile tests, are prohibitively expensive. Therefore, computational augmentation is employed to allow for data-driven approaches. The general framework includes the following four steps: *(0)* characterisation of microstructure images in the data-base by translation-invariant descriptors by MCRpy [1], *(1)* reconstruction of three-dimensional microstructures from the descriptors by MCRpy [1], *(2)* numerical simulations to compute mechanical properties, and *(3)* correlation of all descriptor-property pairs in the data base and prediction of descriptors of potentially improved microstructures. Repeat steps *(1) through (3)* using these new descriptors. This loop is terminated when a microstructure with optimal properties is found.

This framework is applied and demonstrated at the example of a microstructure with hard precipitates of variable position and morphology in a softer matrix. For this purpose, a synthetic initial database of microstructures and corresponding properties is created. Here, mechanical properties, such as yield strength and Young's modulus are considered. Augmenting this small dataset by in silico reconstructed microstructures and their simulated properties allows for deriving improved structure-property linkages and, thus, finding potentially optimal microstructures.

[1] P. Seibert, A. Raßloff, K. A. Kalina, M. Ambati, and M. Kästner, 'Microstructure Characterization and Reconstruction in Python: MCRpy', *Integrating Materials and Manufacturing Innovation*, 2022.

Microstructure generation for discontinuous long fiber-reinforced polymers with curved fiber description and prescribed fiber orientation distribution

Lauff, Celine *(Karlsruhe Institute of Technology, Germany)* 15:20
Schneider, Matti *(Karlsruhe Institute of Technology, Germany)*
Böhlke, Thomas *(Karlsruhe Institute of Technology, Germany)*

Due to their favorable stiffness to weight ratio and the design freedom, discontinuous fiber-reinforced composites are commonly used for lightweight applications. As a consequence of the anisotropy of the fiber reinforcement, the effective properties are anisotropic, as well. Analysing their microstructure with micro-tomography images additionally reveals that the descriptive components vary throughout the component. To obtain the effective properties of such heterogeneous composites, computational multiscale methods complement the oftentimes time-consuming experimental measurements by providing a digital twin of the real microstructures. As starting point a complete representative description of the geometry on the micro-scale is obligatory.

In context of microstructure generation for composites for long fiber-reinforced polymers, the geometry is mainly characterized by the volume fraction of the fibers, their lengths and orientations, as well as their curvature. Fiber orientation data is typically available via fiber orientation tensors of second order. However, for an accurate computation of the effective properties at least the fiber orientation tensor of fourth order is necessary [1] which is obtained by closure schemes [2]. Especially for long fiber-reinforced polymers, analysing 3D-images reveals significant bending. Hence, a curved fiber description is of interesting for generating adequate representative volume elements.

We present an algorithm for generating periodic representative volume elements which take the fiber orientation tensor of fourth order into account. To consider the bending of the fibers, we describe the curvature by discretizing a single fiber as polygonal. To investigate the influence of the curved fiber description and varying fiber orientations on the mechanical behaviour of the microstructure, we compute the effective mechanical properties of the generated microstructures.

References:

[1] V. Müller and T. Böhlke "Prediction of effective elastic properties of fiber reinforced composites using fiber orientation tensors". Composites Science and Technology, Vol. 130, pp. 36-45, 2016.

[2] D. Dray, P. Gilormini, and G. Régnier "Comparison of several closure approximations for evaluating the thermoelastic properties of an injection molded short-fiber composite". Composites Science and Technology, Vol. 67, No. 7-8, pp. 1601-1610, 2007.

Automatic generation of microstructures for materials based on cellulose fibers

Pfeifer, Jan Mirco *(Civil Engineering Mechanics, University of Wuppertal, Germany)* 15:40
Kloppenburg, Greta *(Civil Engineering Mechanics, University of Wuppertal, Germany)*
Kochersperger, Summer *(Chair of Paper Technology and Mechanical Process Engineering, Technical University of Darmstadt, Germany)*
Schabel, Samuel *(Chair of Paper Technology and Mechanical Process Engineering, Technical University of Darmstadt, Germany)*
Dinkelmann, Albrecht *(Competence Center Staple Fibers, Weaving & Simulation, German Institutes of Textile and Fiber Research Denkendorf, Germany)*
Finckh, Hermann *(Competence Center Staple Fibers, Weaving & Simulation, German Institutes of Textile and Fiber Research Denkendorf, Germany)*
Neumann, Johannes *(Civil Engineering Mechanics, University of Wuppertal, Germany)*
Simon, Jaan-Willem *(Civil Engineering Mechanics, University of Wuppertal, Germany)*

Improving our understanding and optimizing the material utilization of materials based on cellulose fibers, such as paper and paperboard, promises high reductions in CO2 emissions and financial costs for various industries (most notably food packaging and building industry).

Due to the complexity of these natural materials, generating such a microstructure is no trivial task. Other works either use simple beam-like structures for the single fibers (cf. [1]) or allow for the fibers to penetrate one another (cf. [2]). In this work, we propose to account for the natural geometry of the single fibers, proper contact areas, and the changing microfibril angles of the fibers (see [3]). These enhancements yield more realistic microstructures, i.e., fiber networks.

In order to automatically generate said fiber networks, a three-step process was implemented. First, fibers were generated and stacked on top of each other. The fibers' dimensions, orientations in space, and microfibril angles varied with prescribed statistical distributions. Next, a representative size was cut out of the stacked fibers. Finally, the fibers were pressed together using a finite element simulation, where the interaction between the fibers was modeled via a cohesive contact formulation. The generated fiber networks were analyzed in terms of criteria for being representative volume elements. For this purpose, numerical homogenization methods were used. Additionally, the numerical models were compared with micro-CT data and macroscopic measurements of paper samples.

The proposed method of generating microstructures for materials based on cellulose fibers improves the efficiency and the quality of the models of previous works. These improvements enable future works to include the generated microstructures in multiscale analyses, which allow for the benefiting industries to optimize their production, and hence minimize consumption of resources.

References:

[1] Tojaga V, Kulachenko A, Östlund S, Gasser TC (2021) Modeling multi-fracturing fibers in fiber networks using elastoplastic Timoshenko beam finite elements with embedded strong discontinuities - Formulation and staggered algorithm. Computer Methods in Applied Mechanics and Engineering 384:113964

[2] Schneider M, Kabel M, Andrä H, Lenske A, Hauptmann M, Majschak J-P, Penter L, Hardt-

mann A, Ihlenfeldt S, Westersteiger R, Glatt E, Wiegmann A (2016) Thermal fiber orientation tensors for digital paper physics. Int J Solids Struct 100-101:234-244
[3] Li Y, Yu Z, Reese S, Simon JW (2018) Evaluation of the out-of-plane response of fiber networks with a representative volume element model. Tappi Journal 17:329-339

S08-05: Multiscales and homogenization

Date: June 1, 2023 08:30-10:30
Room: HSZ/H03

Novel Architectures of Deep Homogenization Neural Networks for Universal Predictions

Eidel, Bernhard *(TU Freiberg, Germany)* 08:30

This contribution proposes a new class of hybrid neural networks for universal prediction of elasticity tensors from homogenization. The very large range of applications of the model in [1] is maintained such as, e.g., a large variety of microstructures, almost arbitrary elastic phase properties, in-built predictions of sharp upper and lower bounds of periodic stiffness to name a few. The architecture however follows a completely different design principle. A thorough error analysis measures the performance of the hybrid model competing with the model in [1].

[1] B. Eidel: Deep CNNs as universal predictors of elasticity tensors in homogenization, Comput. Methods Appl. Mech. Eng., 115741 (2023)

Double U-Net: Microstructure modeling via convolutional neural networks

Lißner, Julian *(Universität Stuttgart, Germany)*
Fritzen, Felix *(Universität Stuttgart, Germany)* 09:10

High performance materials are tuned by optimizing the material on its microscale. Manufacturing processes as well as the required tests during development lead to exorbitant costs and time investments. To improve the efficiency of the design loop, intermediate processes can be substituted by numerical simulations. Nevertheless,due to the representation of the microstructured material via (usually high resolution) images, direct simulations remain computationally costly. One approach to reduce the computational cost is via machine learning.

In microstructure modeling, convolutional neural networks (Conv Nets) have recently gained popularity. One major advantage of Conv Nets is that they operate directly on the image data with no further information required for the prediction. The rise in popularity was amongst others due to the development of the so called U-net, which is a Conv Net layout designed for image predictions based on image inputs, well suited to predict the full field solution of a microstructured image, e.g. the thermal flux. If the data is available, the Conv Net can be expanded to predict any physical behaviour of the microstructured material.

Improvements of the U-net were found by an elaborate extension of the original design and the implementation of a multilevel optimization scheme. Our new model is applied to predict the thermal behaviour of the microstructured material for near arbitrary microstructure input, i.e. by allowing for highly variable microstructure characteristics, input resolutions as well different material phase contrasts, i.e. conducting as well as insulating inclusions.

Continuous Self-Adversarial Training of Recurrent Neural Network Based Constitutive Descriptions

Khedkar, Abhinav Anil *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*
Stöcker, Julien Philipp *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*
Zschocke, Selina *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*
Kaliske, Michael *(Institute for Structural Analysis, Technische Universität Dresden, Germany)*

09:30

Data-driven methods yield advantages in computational homogenization approaches due to the ability to capture complex material behaviour without the necessity to assume specific constitutive models. Neural network based constitutive descriptions are one of the most widely used data-driven approaches in the context of computational mechanics. The accuracy of this method strongly depends on the available data. Additionally, when considering inelastic materials whose constitutive responses depend on the loading history, the accuracy and robustness of the approximation are influenced by the utilized training algorithm. The applied Recurrent Neural Networks exhibit reduced robustness in the presence of errors in the input. When capturing the history dependency by means of previous predicted material responses, occurrences of prediction errors accumulate over several time steps. An approach for achieving enhanced robustness of the predictions is based on extending the initial training dataset by iteratively generating adversarial examples, subjected to perturbations, on the basis of the current prediction errors. In this contribution, a continuous self-adversarial training approach yielding robust recurrent neural network constitutive descriptions for inelastic materials is presented. Compared to the iterative method it is based on, it exhibits significantly improved training efficiency. In order to demonstrate the capabilities of the proposed methods, numerical examples with datasets obtained by Numerical Material Tests on Representative Volume Elements are carried out. Validation of the results is performed using both test load cases from the numerical dataset, as well as application as constitutive model in the Finite Element Method.

FE-NN: efficient scale transition for arbitrary heterogeneous microstructures using neural networks

Stöcker, Julien Philipp *(Technische Universität Dresden, Germany)*
Aldakheel, Fadi *(Leibniz Universität Hannover, Germany)*
Kaliske, Michael *(Technische Universität Dresden, Germany)*

09:50

Numerical modeling and optimization of advanced composite materials can require huge computational effort when considering their heterogeneous mesostructure and interactions between different material phases within the framework of multiscale modeling. Employing Machine Learning methods for computational homogenization enables the reduction of computational effort for the evaluation of the mesostructural behavior while retaining high accuracy. For the description of the heterogeneous structure generally, one unit cell with representative characteristics of the material is chosen, which presents a simplification of the

actual composition. This contribution presents a Neural Network based approach for computational homogenization of composite materials with the ability to consider arbitrary compositions of the mesostructure. Therefore, multiple differently constituted Statistical Volume Elements and their respective constitutive responses are evaluated. Thereby, the naturally occurring fluctuation within the composition of the phases can be considered. Two different approaches using distinct metrics to represent the arbitrary mesostructures are investigated in terms of required computational effort and accuracy. The obtained generalized Neural Network constitutive model is applied in Finite Element Analysis.

Multiscale ANN-based constitutive modeling of multiphase deformable porous materials

Heider, Yousef *(Institute of General Mechanics (IAM), RWTH Aachen University, Germany)* 10:10
Chaaban, Mohamad *(Institute of General Mechanics (IAM), RWTH Aachen University, Germany)*
Sun, WaiChing *(Department of Civil Engineering and Engineering Mechanics, Columbia University, USA)*

Within multiscale simulation of multiphase porous media, the underlying work focuses on artificial neural network (ANN) application to generate material models via supervised machine learning (ML). While feed-forward regression neural networks (FFNN) can be applied for capturing the history-independent material responses, such as for permeability prediction or elasticity models, the recurrent neural networks (RNN) can be used to capture history-dependent responses, such as the retention curve or inelastic material responses. Alternative to RNN, we test in the current contribution the applicability of Conv1D as a type of convolutional neural network (CNN) that operates on one-dimensional data to predict the history-dependent retention model. Moreover, we test RNN accuracy enhancement via the application of deep reinforcement learning (DRL) algorithm, as discussed in [1]. In particular, RNN application allows to automatically discover optimal ANN meta parameters and generates highly accurate trained models. The meta parameters to be discovered include the model architecture (as, e.g., multilayer perceptrons (MLPs), long short-term memory (LSTM), and gated recurrent units (GRUs)), the hyperparameters (as, e.g., number of hidden layers, learning rate, activation function, epochs, batch size, dropout rate), and the chosen strategies (e.g., parameter initialization, data normalization, optimization algorithm). In our approach, the DRL allows for identifying the optimal parameters that result in the highest model score, which is assigned as the prediction accuracy, see, e.g., [1] for more details and references. The database used in the supervised machine learning (ML) relies on lower scale one-and two-phase lattice Boltzmann simulations, applied to deformable and anisotropic representative volume elements (RVEs) of the porous materials as presented in [2]. A special focus in this is on the anisotropy and deformation dependency of the intrinsic permeability tensor as well as the hysteretic nature of the retention model. The presentation will discuss the capability of the ML model to generate a universal permeability model that captures the Darcy and non-Darcy flow on microscale, the enhancement of objectivity of the permeability model, and the

capability of the ML approach to capture the complete and intermediate hysteresis of the retention curves. [1] Heider, Y; Suh H.S.; Sun W. (2021): An offline multi-scale unsaturated poromechanics model enabled by self-designed/self-improved neural networks. Int J Numer Anal Methods;1-26. [2] Chaaban, M.; Heider, Y.; Markert, B. (2022): A multiscale LBM-TPM-PFM approach for modeling of multiphase fluid flow in fractured porous media. Int J Numer Anal Methods Geomech, 46, 2698-2724.

S08-06: Multiscales and homogenization

Date: June 1, 2023 16:00-19:00
Room: HSZ/H03

Nonlinear electro-elastic finite element analysis with physics-augmented neural network constitutive models

Klein, Dominik K. *(TU Darmstadt, Germany)* 16:00
Ortigosa, Rogelio *(TU Cartagena, Spain)*
Weeger, Oliver *(TU Darmstadt, Germany)*

In the last decades, a vast amount of highly specialized metamaterials has been developed and, with advancing requirements in engineering applications, the trend is growing. Often comprised of complex multiphysical microstructures, these materials can be tailored for each specific application. At the same time, this sets a challenge for the mechanical description of such materials, as they behave highly nonlinear. Thus, we envision the use of physics-augmented neural networks, circumventing the current limitations of analytically formulated material models.

In [2], the concept of polyconvex hyperelastic neural network constitutive models [1] was extended towards electro-mechanically coupled material behavior at finite deformations. Using electro-mechanically coupled invariants as inputs for convex neural networks, a polyconvex internal energy is constructed. In this way, the model fulfills common constitutive conditions such as objectivity and ellipticity by construction. Augmenting the neural network with constitutive conditions is not only important to arrive at reliable, i.e., physically sensible model predictions. More than that, it allows for model calibration with small datasets, which are usually only available in engineering applications, e.g., from experimental material characterization tests.

Finally, the model is applied for the finite-element analysis of microstructured electro-active materials [3]. In this way, it is demonstrated how highly flexible neural network constitutive models can be applied for efficient multiscale simulations. Furthermore, the straightforward applicability of the neural network constitutive model in a finite element framework is shown. Lastly, the models are extended towards parametrized material behavior, which is important to account for the often functionally graded nature of metamaterials.

[1] D. K. Klein, M. Fernández, R. J. Martin, P. Neff, O. Weeger. Polyconvex anisotropic hyperelasticity with neural networks. JMPS 159:104703 (2022).
[2] D. K. Klein, R. Ortigosa, J. Martínez-Frutos, O. Weeger. Finite electro-elasticity with physics-augmented neural networks. CMAME 400:115501 (2022).
[3] Nonlinear electro-elastic finite element analysis with neural network constitutive models. In preparation.

Time-adaptive FE²-simulations with deep neural networks for local level evaluation

Tröger, Jendrik-Alexander *(Institute of Applied Mechanics, Clausthal University of Technology, Germany)*
Eivazi, Hamidreza *(Institute of Software and Systems Engineering, Clausthal University of Technology, Germany)*
Hartmann, Stefan *(Institute of Applied Mechanics, Clausthal University of Technology, Germany)*
Wittek, Stefan *(Institute of Software and Systems Engineering, Clausthal University of Technology, Germany)*
Rausch, Andreas *(Institute of Software and Systems Engineering, Clausthal University of Technology, Germany)*

16:20

Nearly all materials, depending on the detail of investigation, possess a heterogeneous micromechanical structure. For example, this is clearly in evidence for modern composite materials that comprise of matrix material and reinforcing fibers. FE^2-simulations with finite elements facilitate the consideration of the internal material structure in macroscale computations. There, a macroscale geometry is discretized with finite elements and the initial boundary-value problem is solved. In contrast to common finite element computations, no material model is evaluated at the macroscopical integration points, but a spatially discretized microstructure. This microstructure, often denoted as representative volume element, is also discretized with finite elements and the particular initial boundary-value problem is solved. The microstructural response are usually homogenized quantities, which are then used on the global, macroscopical level. However, a main drawback of the FE^2-approach are high computational costs due to numerous evaluations of the local level. In this contribution, we apply the FE^2-approach together with deep neural networks to quasi-static problems of solid mechanics. Since deep neural networks can be rapidly evaluated after sufficient training, the homogenized quantities, here stresses and the consistent tangent operator, obtained from the local level are predicted with neural networks leading to a significant speed-up in the overall computational time. First, particular focus is on the algorithmical structure of the FE^2-approach when coupling multiscale finite element simulations and neural networks as predictors. Then, the process of developing a suitable neural network as local predictor is described comprising generation of training data, training of the neural network as well as hyperparameter tuning for the case of nonlinear elastic material behavior on the local level. To accelerate the macroscale computations as much as possible, an efficient implementation and communication between different codes is explained. Lastly, with particular examples it is shown that the application of neural networks is even possible in time-adaptive FE^2-simulations, where the accuracy of the predicted results is crucial.

Descriptor-based microstructure characterization and reconstruction – features and recent progress in MCRpy

Seibert, Paul *(Institute of Solid Mechanics, TU Dresden, Germany)*
Raßloff, Alexander *(Institute of Solid Mechanics, TU Dresden, Germany)*
Kalina, Karl *(Institute of Solid Mechanics, TU Dresden, Germany)*
Safi, Ali *(Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Germany)*
Klusemann, Benjamin *(Institute of Materials Mechanics, Helmholtz-Zentrum Hereon, Germany; Institute of Product and Process Innovation, Leuphana University of Lüneburg, Germany)*
Kästner, Markus *(Institute of Solid Mechanics, TU Dresden, Germany; Dresden Center for Computational Materials Science, TU Dresden, Germany; Dresden Center for Fatigue and Reliability, TU Dresden, Germany)*

16:40

Microstructure Characterization and Reconstruction (MCR) allows for (i) generating a plausible 3D computational domain from 2D information like a microscopy image, (ii) generating a set of statistical volume elements from a single representative example and (iii) augmenting microstructure datasets by sampling and interpolating in the descriptor space and subsequently reconstructing the corresponding structures. Two classes of reconstruction algorithms, descriptor-based and machine learning-based approaches, are distinguished and their advantages and disadvantages for computational materials engineering are compared. After a formulation of the descriptor-based optimization problem, MCRpy is presented [1], a recently developed modular and extensible open-source software that facilitates microstructure characterization and descriptor-based reconstruction. MCRpy enables flexible combinations of descriptors, loss functions and optimizers and therefore implements a spectrum of reconstruction approaches ranging from the classical Yeong-Torquato algorithm to recent, gradient-based formulations [2, 3]. Recent developments comprise novel descriptors, different levels of expressivity of the same descriptors as a performance-accuracy trade-off as well as developments towards texture reconstruction. Finally, a validation is presented in order to demonstrate the utility of a realistic microscale domain in homogenization and multiscale modeling.

[1] Seibert, Raßloff, Kalina, Ambati, Kästner, Microstructure Characterization and Reconstruction in Python: MCRpy, IMMJ, 2022.
[2] Seibert, Ambati, Raßloff, Kästner, Reconstructing random heterogeneous media through differentiable optimization, COMMAT, 2021.
[3] Seibert, Raßloff, Ambati, Kästner, Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization, Acta Materialia, 2022.

Stress and strain partitioning in nanocrystalline thin films using atomistic simulations and statistical machine learning

Prakash, Arun *(TU Bergakademie Freiberg, Germany)*

17:00

How does a macroscopic applied stress or strain field distribute or partition into individual grains of a polycrystalline material? This is indeed a long-standing question in the field of crystal plasticity. The well-known Taylor and Sachs models provide bounds in this regard, with the Taylor model enforcing iso-strain and the Sachs model enforcing iso-stress; the response of real materials lies somewhere in between. In this work, we investigate the partitioning of

continuum fields, particularly strain fields in nano(poly)crystalline thin films, which find potential applications in many technologically relevant fields. These films constitute interesting material systems since they often display enhanced mechanical properties in comparison to their bulk counterparts. Atomistic simulations are performed on such thin film structures to analyze the deformation behavior under tensile loading conditions. We then apply statistical machine learning algorithms to understand the inhomogeneity in field distributions. Specifically, we look into the distribution of total strain, elastic strain and microrotation fields in individual grains in the polycrystalline structure. The results show a lognormal-like distribution of the elastic strain which is in contrast to the normal distribution observed for coarse-grained materials. Whilst the distribution of the elastic strain is unimodal, the distribution of total strain (and microrotation) is multimodal consisting of distinct peaks. We use a Gaussian mixture model to identify these peaks, and furthermore, correlate the individual peaks with deformation events occurring in individual grains. The proposed methodology is a general framework that can be applied to other simulation techniques as well. Finally, we discuss the results obtained in the context of bridging length scales towards higher scale simulations.

Multiscale modeling of additively manufactured shell lattice metamaterials

Shojaee, Mohammad *(Cyber-Physical Simulation Group, Department of Mechanical Engineering, Technical University of Darmstadt)* 17:20
Valizadeh, Iman *(Cyber-Physical Simulation Group, Department of Mechanical Engineering, Technical University of Darmstadt)*
Klein, Dominik *(Cyber-Physical Simulation Group, Department of Mechanical Engineering, Technical University of Darmstadt)*
Sharifi, Peyman *(Department of Mechanical Engineering,Shiraz University, Iran)*
Weeger, Oliver *(Cyber-Physical Simulation Group, Department of Mechanical Engineering, Technical University of Darmstadt)*

In recent years, the development of additive manufacturing techniques has led to the fabrication of functionally graded lattices with customized mechanical properties. The lattices are made up of a repeating pattern of beams, plates, or thin-walled, shell-like geometries. In this regard, triply periodic minimal surfaces (TPMSs) have interesting geometric and mechanical properties to use in wide applications with efficient design. However, there are still many unanswered questions about the mechanical behavior of shell lattices, including stability, deformability, and response to external forces. To tackle the issue, a microscale simulation is present to homogenize the effective mechanical properties of different geometrical parameters of the Schwartz primitive unit cell. Furthermore, the microscale simulations are validated through experimental comparison tests of samples provided by 3D printing. Using the large data set provided by these simulations, a parametric material model based on a physics-enhanced neural network is employed to predict the constitutive behavior of a graded elastic solid structures at any arbitrary material point. Finally, macroscale models made of graded shell lattices in the framework of linear elasticity are studied to show the reliability and performance of the proposed approach. In this regard, the differential quadrature method (DQM) as an efficient and low-cost computational tool is used to discretize the governing equations

and the related boundary conditions. Lastly, the convergence and accuracy of the static multiscale analysis results based on the present approach at the finite deformation continuum level are discussed.

Adaptive MOR techniques for non-linear FE simulations of unitcells

Özmen, Yasemin *(University of Duisburg-Essen, Germany)*
Niekamp, Rainer *(University of Duisburg-Essen, Germany)*
Nigro, Paulo S. B. *(Akselos S. A., Switzerland)*
Schröder, Jörg *(University of Duisburg-Essen, Germany)*

17:40

Model order reduction strategies have undergone extensive development and use in the field of mechanical simulations in recent years. Methods include proper generalized decomposition (PGD), proper orthogonal decomposition (POD), and hyper-reduction (HR), to mention a few. These kinds of techniques are also applied to numerical simulations including non-linearities. For example, it is suggested in [1] to apply a POD method to subdomains with approximative linear behavior. The authors in [2] develop virtual inclusions and conduct a HR prediction on those. Reduced order techniques are furthermore used in the context of finite element simulations for multiscale modeling. Due to the enormous computing effort of such problems, a significant area of research and application have emerged for this field. For instance, the authors in [3] compute an appropriate lower dimensional POD-subspace for various micro-problem deformation modes in an offline stage, which then speeds up the microscale computations during the multiscale simulation. Or, as suggested in [4], local RB for the dynamically updated micro-problems in each Gauss point could be used together with HR, to control the decreased dimension.

An adaptive POD approach for small strain elasto-plastic material behavior is demonstrated in the shown work which is based on the formulations in [5]. The choice of a suitable reduced basis to capture the overall non-linearities of the problem's response without the need of an offline stage is one of the primary challenges within this work. This is accomplished by implementing an adaptive selection method, which gives the algorithm the necessary adaptability to change the reduced basis as needed. The presentation includes numerical simulations with examples from multiscale analysis.

[1] A. Robens-Radermacher and S. Reese, Model reduction in elastoplasticity: proper orthogonal decomposition combined with adaptive sub-structuring, Int. J. Comp. Mech., Vol. 54, 677-687, (2014).
[2] D. Ryckelynck et al., Hyper-reduced predictions for lifetime assessment of elasto-plastic structures, Meccanica, Vol. 51, 309-317, (2016).
[3] A. Robens-Radermacher et al., Displacement-based multiscale modeling of fiber-reinforced composites by means of proper orthogonal decomposition, Adv. Model. Simul. Eng. Sci., Vol. 3, 2213-7467, (2016).
[4] W. He et al., In situ adaptive reduction of nonlinear multiscale structural dynamics models, Int. J. Numer. Methods Eng., Vol. 121, 4971-4988, (2022).
[5] P. S. B. Nigro et al., An adaptive model order reduction with Quasi-Newton method for nonlinear dynamical problems, Int. J. Num. Meth. Engng., Vol. 106: 740-759, (2016).

Computational homogenization by the monolithic hyper ROM FE² method using clustered training

Lange, Nils *(Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany)*
Hütter, Geralf *(Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany; Institute of Civil and Structural Engineering, BTU Cottbus-Senftenberg, Germany)*
Kiefer, Bjoern *(Institute of Mechanics and Fluid Dynamics, TU Bergakademie Freiberg, Germany)*

18:00

The usage of numerical homogenization tools in order to obtain the mechanical behavior at a higher length scale is commonly established and widely applied. The most general approach is the utilization of the finite element method on both scales, known as the FE^2 method. The high generality comes along with a high computational effort, usually leading to the necessity of finding approximative reduction methods. In order to assess the eligibility of these methods, at least three factors must be taken into account:

(I) online effort (simulation of the structural problem)
(II) offline effort (training data generation)
(III) problem specific adaptation effort

The most obvious criterion is an appreciable computing time reduction when simulating the structural problem. However, from a practical standpoint, it is also necessary to set the training effort and the effort of adapting a general method to the needs of a specific problem in relation to the online time.

To address these points, we present a hyper integrated reduced order modeling FE^2 scheme with monolithic solution strategy at large deformations. This approach is shown to yield a considerable reduction of online simulation time. Additionally, a specific, clustered training strategy drastically lowers the training costs. Representative numerical examples are presented, which include three dimensional problems with elastic-plastic deformations of porous microstructures, creep in ceramic foams, among others, in order to show the wide applicability at minimal effort of adapting the method to a specific problem.

Asymptotic Reduction for Thin Porous Materials with a Linearized Corrector

Armiti-Juber, Alaa *(University of Stuttgart, Germany)*
Ricken, Tim *(University of Stuttgart, Germany)*

18:20

The dynamical behavior of saturated, thin, porous materials, such as soil, filters, fuel cells, and some biological tissues such as cartilage, is typically described using coupled, nonlinear partial differential equations (PDEs). High-fidelity simulations of these PDEs require advanced numerical methods and might, therefore, be time-consuming. Despite the huge advances in computational algorithms and computer chips, this can be problematic for many applications, such as design optimization, model-based predictive control, or clinical-time constraints.

Thin, porous materials are, however, of high aspect-ratio, such that the dynamics in the small-scale direction reach equilibrium much faster than in the large-scale directions. This property has been utilized to construct knowledge-driven reduced-order models using methodologies such as vertical averaging, asymptotic analysis [1,2], and rigid convergence analysis [3]. The

resulting reduced model is typically a combination of a low-dimensional (limit) model, describing the effective dynamics in the large-scale directions, and a full-dimensional (corrector) model that recaptures the less effective dynamics in the small-scale direction.

The asymptotic reduction method is applied in [2] to thin materials undergoing infinitesimal deformations, where the full biphasic model is considered in the actual configuration. We apply the method to the full biphasic model pulled back in the reference configuration. Then, the resulting reduced model consists of a nonlinear limit model and a linear corrector model. This model has improved computational efficiency as the linearization step using the Newton method is only required for the low-dimensional limit model. We investigate the model's validity for thin, porous materials under two loading scenarios; firstly, load is applied in the large-scale direction, and secondly load is applied in the small-scale direction.

[1] Armiti-Juber, A., and Rohde, C. (2019): Computational Geosciences.

[2] Armiti-Juber, A. and Ricken, T. (2022): Archive of Applied Mechanics.

[3] Armiti-Juber, A. (2022): Mathematical Methods in the Applied Sciences.

Two-scale methods at finite elasticity based on the Virtual Element Method

Böhm, Christoph *(Institute of Continuum Mechanics, Leibniz University Hannover, Germany)*
Hudobivnik, Blaž *(Institute of Continuum Mechanics, Leibniz University Hannover, Germany)*
Marino, Michele *(Department of Civil Eng. and Computer Science, University Rome Tor Vergata, Italy)*
Korelc, Jože *(Faculty of Civil and Geodetic Engineering, University of Ljubljana, Slovenia)*
Wriggers, Peter *(Institute of Continuum Mechanics, Leibniz University Hannover, Germany)*

18:40

The field of micromechanics and computational homogenization is undergoing continuous developments and attracts attention throughout many research groups. Besides material-models, that can predict complex material behavior, particular attention is paid to schemes that being able to simulate macroscopic load application, coupled with the solution of boundary value problems at lower length scales, compare for example the FE2 -method in [4]. While providing a quite general scheme that holds consistency from a theoretical background, those two-scale schemes suffer from the fact of being computationally expensive due to their scaling of the amount of microscopic problems with the number of integration points, that is for example 8 Gauss points per element for a 3D hexahedral element on macroscopic length scales. Improvement to this can be made on both of the length scales by using the Virtual Element Method (VEM), that has recently provided evidence for superior computational homogenization behavior in e.g. [1, 2] or for non-linear applications in [3]. One key ingredient of using VEM is the reduction of the element number at microscopic length scales while restoring still an accurate result for homogenized properties. This gains attraction for the application of a mixed FE-VE scheme for two-scale methods. However, low order VE-approaches exhibit only one integration point. An immediate consequence of this is for the use of VE2 methods, that the number of micro-problems scales directly with the number of macroscopic

elements. This makes VE2 be able to reduce computational costs, when compared to established schemes such as FE2. The code is derived and optimized by the AceGen-tool from [5].
The authors acknowledge financial support to this work by the DFG Collaborative Research Centre CRC 1153 "Process chain for the production of hybrid high-performance components through tailored forming", project no. 252662854.

[1] M. Marino, B. Hudobivnik, P. Wriggers. Computational homogenization of polycrystalline materials with the Virtual Element Method. Computer Methods in Applied Mechanics and Engineering, 355:349-372, 2019.
[2] C. Böhm, B. Hudobivnik, M. Marino, P. Wriggers. Electro-magneto-mechanically response of polycrystalline materials: Computational Homogenization via the Virtual Element Method. Computer Methods in Applied Mechanics and Engineering, 380:113775, 2021.
[3] P. Wriggers, B. Hudobivnik. A low order virtual element formulation for finite elasto-plastic deformations. Computer Methods in Applied Mechanics and Engineering, 327:459-477, 2017.
[4] J. Schröder, M.-A. Keip. Two-scale homogenization of electromechanically coupled boundary value problems. Computational mechanics, 50(2):229-244, 2012.
[5] J. Korelc, P. Wriggers. Automation of Finite Element Methods. Springer, 2016.

S08-07: Multiscales and homogenization

Date: June 2, 2023 08:30-10:30
Room: HSZ/H03

Multidimensional numerical relaxation in continuum damage mechanics

Balzani, Daniel *(Chair of Continuum Mechanics, Ruhr-Universität Bochum, Germany)* 08:30
Köhler, Maximilian *(Chair of Continuum Mechanics, Ruhr-Universität Bochum, Germany)*
Neumeier, Timo *(Institute of Mathematics, University of Augsburg, Germany)*
Peter, Malte A. *(Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg, Germany)*
Peterseim, Daniel *(Institute of Mathematics & Centre for Advanced Analytics and Predictive Sciences (CAAPS), University of Augsburg, Germany)*
Wiedemann, David *(Institute of Mathematics, University of Augsburg, Germany)*

In this talk, we focus on the simulation of a pseudo-time-incremental damage model in the finite strain setting. Due to the damage evolution, the incremental strain energy densities become non-convex and, thus, the direct numerical simulation suffers from mesh dependence and stability issues. To overcome these drawbacks, we establish the relaxed model and discuss feasible algorithms for the approximation of semi-convex hulls, like the rank-one convex envelope, in higher spatial dimensions. The use of weaker convexity notions enables the relaxed model to capture strain-softening of the material while providing mesh-independent approximations simultaneously. An interpretation in terms of microstructural damage evolution is given, based on the information gained in the convexification process.

Multiscale simulation of fracture in complex materials under impact loads

Knobloch, Hannah *(Technische Universität Dresden, Germany)* 08:50
Loehnert, Stefan *(Technische Universität Dresden, Germany)*

Within the construction sector, an increasing number of complex materials is being developed to build new and support old infrastructure. An example is fiber-reinforced concrete, which can be applied as a reinfocing layer to protect existing conrete structures. In order to increase its tensile strength and ductility, short fibers are embedded into a fine-grained concrete matrix, making it particularly suitable to withstand impact loads. The simulation of such complex materials is difficult, since several effects must be considered, such as microscopic cracks, which expand, branch and coalesce, and lead to complicated fracture networks on a structural level. Moreover, inertia effects must be considered when regarding impact loads. For the simulation of these occurring processes, an efficient multiscale framework must be developed that can handle localization phenomena as well as dynamic effects. To achieve this, features of the Multiscale Projection Method as well as the Generalized Finite Element Method with global-local enrichment are used. Both methods share the basic idea that within certain areas of interest microscopic aspects are included into the coarse scale simulation through an additional fine scale analysis. This is accomplished by performing a separate simulation, permitting the incorporation of a more accurate material model or the explicit representaion of

fibers and micro cracks. The scales are coupled in a concurrent way - first the displacements obtained from the coarse scale simulation are employed as boundary conditions for the fine scale simulation. Then the fine scale problem is solved, where the complex fracture behavior is represented with the help of the phase-field method. Now the resulting displacement field can be used to construct a numerical enrichment that reproduces the displacement jump across the crack on the coarse scale. Additionally, the degradation resulting from the phase-field formulation on the fine scale is projected back to the coarse scale, in order to account for the loss of stiffness within damaged material.
As the incorporation of dynamic effects and fracture can be problematic within multiscale simulations due to spurious wave refelctions at domain boundaries and crack surfaces, simplified 1D investigations are conducted, in order to gain a deeper understanding of the complex effects of this method. In the end it is shown that with the help of this multiscale simulation method, complex materials such as fiber-reinforced concrete can be modeled in 3D efficiently and accurately.

Influence of homogenization scheme and material morphology on multiscale simulation of concrete damage

Vu, Giao *(Institute for Structural Mechanics, Ruhr-Universität Bochum, Germany)*
Timothy, Jithender J. *(Centre for Building Materials (cbm), Technical University of Munich)*
Meschke, Günther *(Institute for Structural Mechanics, Ruhr-Universität Bochum, Germany)*
09:10

Identifying and preventing damage in concrete structures at an early stage of material degradation can significantly reduce costs associated with the maintenance and repair of concrete infrastructure. Weak material degradation, such as load-induced microcracking, is a precursor of localized damage (macrocracking) in concrete structures. Therefore, simulations of diffuse microcracking can provide insights on the factors governing damage in concrete. To this end, the influence of the modelling assumptions in the multiscale model for concrete proposed in [1] is investigated. The aforementioned multiscale model takes into account the concrete mesostructure comprising of coarse aggregates embedded in a mortar matrix [2]. Damage evolution is modelled as the growth of pre-existing microcracks whose propagation is governed by Linear Elastic Fracture Mechanics. Localization and Homogenization operations are performed by means of cluster based Lipmann-Schwinger solver and Continuum Micromechanics, respectively. In this contribution, we investigate the influence of the homogenization scheme (e.g. Mori-Tanaka, Interaction Direct Derivative), the clustering algorithm, the mesoscopic internal structure as well as microcrack morphology on the macroscopic response of concrete. Using experimental data, a suitable implementation for simulating diffuse damage in concrete is presented and discussed.

[1] Vu, G., Diewald, F., Timothy, J. J., Gehlen, C., & Meschke, G. (2021). Reduced Order Multiscale Simulation of Diffuse Damage in Concrete. Materials, 14(14), 3830.
[2] Holla, V., Vu, G., Timothy, J. J., Diewald, F., Gehlen, C., & Meschke, G. (2021). Computational generation of virtual concrete mesostructures. Materials, 14(14), 3782.

Finite Element Study of Pore Collapse and Densification in Silica Aerogels using Representative Volume Elements

Xiong, Weibo *(Department of Continuum Mechanics, RWTH Aachen University, 52062 Aachen, Germany;)*
Abdusalamov, Rasul *(Department of Continuum Mechanics, RWTH Aachen University, 52062 Aachen, Germany;)*
Itskov, Mikhail *(Department of Continuum Mechanics, RWTH Aachen University, 52062 Aachen, Germany;)*
Milow, Barbara *(Institute of Materials Research, German Aerospace Center, 51147 Cologne, Germany;)*
Rege, Ameya *(Institute of Materials Research, German Aerospace Center, 51147 Cologne, Germany;)*

09:30

Aerogels are porous materials characterized by low thermal conductivity, bulk densities, and sound velocities, but with limited applications due to poor mechanical properties. This study aims to better understand the mechanical properties of aggregated silica aerogels by examining the microstructural connectivity and investigating the pore collapse and densification under uniaxial compression. The inter-particle connectivity was generated using the diffusion-limited cluster-cluster aggregation (DLCA) algorithm. Each particle connection is modeled by elasto-plastic beam elements by considering their damage and contact. The mechanical behavior is analyzed in both the elastic and inelastic regimes using representative volume elements (RVEs) subject to periodic boundary conditions. The model was correlated with experimental compression test data to validate the simulation results. With increasing compressive strain, load transition between multiple backbone paths appears in the network structure. Thus, the simulation model provides a good insight into fracture progression. It also allows to examine the influences of model parameters and in particular to evaluate the power law relationship between the elasticity modulus and porosity of aerogels.

MULTISCALE MODELING OF COMPRESSIBLE CEMENTITIOUS MATERIALS

Iskhakov, Tagir *(Ruhr-Universität Bochum, Germany)*
Timothy, Jithender J. *(Technical University of Munich, Germany)*
Meschke, Günther *(Ruhr-Universität Bochum, Germany)*

09:50

Tunnel constructions under difficult geological conditions such as expansive rocks (e.g., Opalinus Clay) may undergo deterioration processes leading eventually to complete failure of the structure. This can potentially be prevented by incorporating around the tunnel lining a deformable protective layer made of highly compressible cementitious composite materials. Such materials are characterized by their deformation capacity achieved by introducing into the mix various weak inclusions (e.g., air voids, expanded polystyrene (EPS) beads, expanded glass beads). These individual constituents govern the microstructure of the composite material and its overall properties. For a case of specific ground conditions, the design of the composite cementitious materials can be supported by a computational framework. A multiscale model combining the continuum micromechanics and a voxel based approach is used to predict the composite material behavior under compression. The compaction of the material under compressive loading is represented by an injection of the eigenstrains into the

voxels. At the microscale, the damage criterion in the vicinity of the individual composite constituents is formulated by means of the exterior point Eshelby solution. Model predictions for the behavior of selected composite mixes under compression are compared with experimental observations.

Two-scale modeling of the viscosity of fiber suspension

Sterr, Benedikt *(Karlsruhe Institute of Technology (KIT), Germany)*
Schneider, Matti *(Karlsruhe Institute of Technology (KIT), Germany)*
Böhlke, Thomas *(Karlsruhe Institute of Technology (KIT), Germany)*

10:10

The viscosity of fiber suspensions plays an important role in manufacturing fiber reinforced composite components, for example in injection and compression molding. Therefore, an accurate understanding of the viscous properties of fiber suspensions is important for appropriate industrial application. Taking microstructural parameters into account, Fast Fourier Transform (FFT) based simulations enable high fidelity homogenization of viscous properties of fiber suspensions [1], thus laying the foundation for computational two-scale strategies. Previous work [1] on FFT-based two-scale strategies has been limited to the assumption of a Newtonian polymer melt. However, polymer melts typically show non-Newtonian behavior. Here we investigate scale transition in the viscosity of fiber suspensions using the Cross-WLF [2,3] material model and an extended computational method. We study the influence of loading direction and magnitude, as well as microstructural parameters on the effective viscosity of fiber suspensions with a non-Newtonian matrix. We compare our results to effective viscosities of fiber suspensions with a Newtonian matrix.

[1] Róbert Bertóti, Daniel Wicht, Andrew Hrymak, Matti Schneider, and Thomas Böhlke. A computational investigation of the effective viscosity of short-fiber reinforced thermoplastics by an FFT-based method. European Journal of Mechanics - B/Fluids (2021), 90: 99-113.
[2] Malcolm M. Cross. Rheology of non-Newtonian fluids: a new flow equation for pseudoplastic systems. Journal of colloid science (1965), 20(5), 417-437.
[3] Malcolm L. Williams, Robert F. Landel, and John D. Ferry. The temperature dependence of relaxation mechanisms in amorphous polymers and other glass-forming liquids. Journal of the American Chemical society (1955), 77(14), 3701-3707.

S08-08: Multiscales and homogenization

Date: June 2, 2023 11:00-13:00
Room: HSZ/H03

On the three-dimensional numerical analysis of residual stresses on two scales in hot bulk forming parts

Hellebrand, Sonja *(University of Duisburg-Essen, Germany)* 11:00
Brands, Dominik *(University of Duisburg-Essen, Germany)*
Schröder, Jörg *(University of Duisburg-Essen, Germany)*

Current research focuses on the induction of residual stresses in a component during its manufacturing process, which shows a significant impact on the final component's properties. For instance, compressive residual stresses in regions that undergo tensile loading can prevent crack initiation or crack growth and, as a consequence, can lead to an improved service life. Especially, hot bulk forming processes offer a good possibility to adapt the residual stresses during the component's manufacturing since it enables to exploit interactions of thermal, mechanical and metallurgical kind. Such processes are divided into three steps: heating, forming and cooling. Considering the Cr-alloyed steel 100Cr6, the heating to above 1000°C leads to an austenization of the material. Afterwards, the forming induces plastic deformation in the material. Finally, the subsequent cooling of the component evokes a phase transformation from the austenitic parent phase to different product phases, e.g. a fast cooling in water leads to a diffusionless martensitic phase transformation. As a result of the phase transformation, microscopic and macroscopic residual stresses occur in the component.

In order to analyze these stresses and for a cost and time efficient process design to obtain targeted residual stress distributions, a combination of experimental measurements and numerical simulations provide a good toolbox. Microscopic characteristics such as the phase transformation motivate a multi-scale investigation, in which residual stresses of different types (macroscopic and microscopic) can be depicted, see [1,2]. Thus, in this contribution the focus lies on the cooling of a cylindrical specimen made from the steel 100Cr6 as hot bulk forming part. Therefore, in a first step, a single-scale finite element simulation is carried out to examine macroscopic (residual) stress distributions. Afterwards, two-scale finite element simulations are applied for certain points of the geometry, utilizing the FE^2 approach, which resolves the microscale based on a representative volume element, see [3]. Thereby, microsopic (residual) stresses are obtained which will be discussed.

Downwind and upwind approximations for mesh- and model adaptivity of elasto-plastic composites

Tchomgue Simeu, Arnold *(University Paderborn, Germany)* 11:20
Mahnken, Rolf *(University Paderborn, Germany)*

The use of heterogeneous materials, such as composites with Prandtl-Reuss type material laws, has increased in industrial praxis making finite element modeling with homogenization techniques a well-accepted and often unavoidable tool. These methods are very advantageous to account for microstructural mechanisms which can be related to nonlinearities

and time-dependency due to elasto-plasticity behavior. However, their advantages are diminished by increasing computational demand. The present contribution deals with the balance of accuracy and numerical efficiency of nonlinear homogenization associated with a framework of goal-oriented adaptivity which takes into account error accumulation over time. To this end, model adaptivity of homogenization methods is coupled to mesh adaptivity on the macro scale. Therefore, a fully coupled adaptive strategy is established to control simultaneously model and spatial discretization errors of the finite element method. The new proposed adaptive procedure is driven by a goal-oriented a posteriori error estimator based on duality techniques using downwind and upwind approximations. Duality techniques originated from the dual-weighted residual method and allow a link between the dual form of the primal problem and a user-defined quantity of interest. Due to nonlinearities and time-dependency of the plasticity, the estimation of error transport and error generation is obtained with a backward-in-time dual method despite a high demand on memory capacity. In this contribution, the dual problem is solved with a forward-in-time dual method that allows estimating the full error during the resolution of the primal problem without the need for extra memory capacity. In addition, the new proposed framework of goal-oriented adaptive with downwind approximation is faster than with the upwind approximation. Finally, several numerical examples in this paper illustrate the effectiveness of the proposed adaptive approach based on downwind approximations in comparison to upwind approximations.

Extension of a shell-like RVE model to represent transverse shear effects in textile reinforced composites

Khattabi, Omar *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*
Landgraf, Ralf *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*
Ihlemann, Jörn *(Chair of Solid Mechanics, Chemnitz University of Technology, Chemnitz, Germany)*
11:40

Textile reinforcements have long been used in shell-like components like tires, belts, hoses and, in particular, air spring bellows. These bellows consist of a certain number of cords embedded in soft rubber, resulting in high membrane stiffness to absorb tensile forces and low resistance to changes in curvature. The embedded cords are produced by twisting multifilament yarns. Modelling and simulation of bellows is a challenging task. Thereby, the complex internal geometry, large deformations as well as the strongly anisotropic and nonlinear material behavior have to be taken into account in a computationally efficient manner. One approach is the application of multiscale analyses in conjunction with representative volume elements (RVE). Within this study, a through-thickness RVE based on in-plane periodic microstructures is applied (see, for example, [1]). Therein, the local behavior of the cords is represented by an anisotropic constitutive model that regards directions and mechanical properties of filaments, which result from a previous cord twisting simulations.

In this contribution, an extension of the classical periodic boundary conditions is presented, which considers curvature, pressure load, and, in particular, transverse shear. The RVE is used to simulate the stresses and strains on in cord-rubber composites under realistic load

conditions. Moreover, it is employed for homogenizing the mechanical behavior and, thus, for developing a suitable constitutive model for shells.

[1] Donner, D. (2017). FEM-basierte Modellierung stark anisotroper Hybridcord-Elastomer-Verbunde. PhD Thesis, TU Chemnitz.

Multiscale Modelling of Concrete Reinforced with Shape Memory Alloys: An Investigation into the Mechanical Properties of High-Performance Concrete

Tabrizikahou, Alireza *(Institute of Building Engineering, Poznan University of Technology, Poland)*
Kuczma, Mieczyslaw *(Institute of Building Engineering, Poznan University of Technology, Poland)*

12:00

A multiscale modelling technique is defined in this research to analyse the mechanical behaviour of concrete reinforced with shape memory alloys (SMAs), to establish high-performance concrete (HPC) with improved properties such as stiffness, energy dissipation, and hysteresis. The numerical model was created utilizing the Abaqus program, and the user-defined function UMAT was written in Python and Fortran. To capture the micro-scale behaviour of the concrete-SMA composite material, the model included periodic boundary conditions and we used the principle of representative volume element (RVE). The micro-scale response was then homogenized to assess the material's macro-scale responses. The concrete damage plasticity (CDP) model was also incorporated into the model to account for the behaviour of the concrete under stress. The research was carried out utilizing a combination of experimental and numerical techniques. Concrete specimens reinforced with SMAs were utilized by the researchers to obtain data on the material's mechanical characteristics. This information was then utilized to verify the numerical model of HPC generated using the finite element approach. The numerical model findings indicated that incorporating SMAs in concrete resulted in increased energy dissipation and stiffness, as well as a reduction in deterioration. The presented contribution is an innovative multiscale modelling technique that was utilized to evaluate the behaviour of shape memory alloy reinforced concrete. This comprehensive research on the subject of high-performance concrete uses Abaqus, Python, and Fortran for UMAT, RVE, homogenization, and the CDP model for concrete. The results of numerical simulations for test problems will be presented at the conference.

Variationally consistent computational homogenization of chemo-mechanical properties of structural battery electrode materials

Rollin, David *(Technische Universität Braunschweig, Germany)*
Larsson, Fredrik *(Chalmers University of Technology, Sweden)*
Runesson, Kenneth *(Chalmers University of Technology, Sweden)*
Jänicke, Ralf *(Technische Universität Braunschweig, Germany)*

12:20

The importance of Li-ion batteries for many different applications is driving the development and optimization of different types of batteries. For this, various multiphysics processes on multiple length scales need to be taken into account. A promising approach to achieve mass savings is the concept of a structural battery. This type of battery stores energy as well as it bears mechanical loads. Thus, the mechanical properties and their interactions with the

electro-chemical processes need to be considered. For a structural Li-ion battery, the volume change of the electrode material due to lithium storage is a crucial aspect. There are different approaches to realizing a structural battery. One of them is to produce a carbon fiber reinforced polymer as a multi-functional composite material. In this case, the carbon fibers serve as negative electrode as well as mechanical reinforcement and current collector in both electrodes. The positive electrode can be designed as a coating on some of the fibers. Such a coating material typically consists of particles, for storing the lithium, embedded in a porous polymer matrix saturated with a liquid electrolyte. For this type of microstructure, our aim is to develop a model describing the chemo-mechanical coupling mechanisms. This study uses artificially generated microstructures as no 3D imaging data is available. To investigate the processes across the scales, the concept of variationally consistent computational homogenization is applied. Our starting point is a linearized chemo-mechanical model which will be extended to account for reaction kinetics on the particle surfaces. First order homogenization is applied to derive a two-scale problem from the fine-scale model.

Influence of grain boundaries on the overall diffusivity in polycrystalline solids

Scholz, Lena *(University of Stuttgart, Germany)* 12:40
Fritzen, Felix *(University of Stuttgart, Germany)*
Grabowski, Blazej *(University of Stuttgart, Germany)*

Major progress in battery technology is a key to the decarbonization of industry and everyday life. In All-Solid State Lithium Ion Batteries (ASSLIBs) the liquid electrolyte of conventional Lithium ion batteries is replaced by a polycrystalline solid-state electrolyte. It seems promising that ASSLIBs might outperform conventional Lithium ion batteries with respect to capacity, operational safety and charging performance. Therefore, an in-depth understanding of the multiphysical multiscale effects within the solid-state electrolyte is subject of research across various disciplines. However, grain boundary effects and the chemo-mechanical coupling have been rarely investigated concurrently in this context. The details of the polycrystalline structure are often neglected or only considered under strong assumptions such as isotropy. If effects on small scales are taken into account, computational costs often restrict the dimensions of the considered domain.

Our approach aims to describe Li^+ diffusion in the solid-state electrolyte as well as its mechanical behavior and the impact of operation temperature together with the strong coupling between these phenomena. The consideration of the fully resolved crystalline structure allows us to find a microscopic description that accounts for diffusion along as well as across grain boundaries. It is governed by differing and potentially anisotropic diffusion coefficients in bulk and grain boundary domains gained from ab initio calculations. For the bulk a chemo-mechanical coupling is assumed which is strongly interlinked with the diffusion properties. By means of homogenization an effective model on the mesoscale is derived based on a periodic reference volume element (RVE).

Using the hybrid bulk-interface diffusion model, the contribution of the grain boundary to the overall diffusivity can be studied quantitatively. The grain size has been found to have a significant impact on the overall diffusivity, as recently described, e.g., by Dawson and Islam[1]. However, the atomistic simulations used in the mentioned study go along with massive computational demands, thereby limiting the size of the studied cells considerably. We aim towards overcoming these limitations by using data-integrated techniques for the consideration of grain boundary diffusion that depends on the misorientation of neighboring grains. This will facilitate in silico exploration of microstructures and their implications on larger scales which, at a later stage, can be used to design improved batteries.

[1] J.A. Dawson and M.S. Islam, "A Nanoscale Design Approach for Enhancing the Li-Ion Conductivity of the Li10GeP2S12 Solid Electrolyte," in ACS Materials Letters, vol. 4, pp. 424-431, 2022

S08-09: Multiscales and homogenization

Date: June 2, 2023 16:00-18:00
Room: HSZ/H03

Multi-scale modelling and homogenization of weakly cemented granular mixtures

Jiang, Yupeng *(leibniz universität hannover, Germany)* 16:00

Granular mixtures — a composite state of continuum and discrete materials - are ubiquitous in modern industries, including food processing, concrete manufacturing, and soil treatments. A high-fidelity numerical method is critical for characterizing the local heterogeneity of granular mixtures and constructing a reliable homogenization. Existing approaches for simulating the granular mixtures have relied on either a purely discrete or continuum method. Both approaches, however, suffer from computational stability and efficiency due to distinct differences in components' size and material modulus. In this paper, we adopt a hybrid continuum-discrete approach, material-point discrete-element methods (MP-DEM), to simulate granular mixtures in a weakly cemented state. We simulate cement matrices, a deformable continuum, using MPM, and handle cemented particles with high stiffness via DEM. We first demonstrate the solver's capability for capturing complicated and unique behaviours, such as shear and particle segregation, against experimental data. Then, we provide a computational framework for homogenization in weakly cemented granular mixtures based on the numerical results. Results have shown that the hybrid solver MP-DEM can adequately reflect the material heterogeneity of granular mixtures on the mesoscale and provide insights for constructing the representative volume element (RVE) on the macro-scale.

Investigating the impact of deformation on foam permeability through CT scans and the Lattice-Boltzmann method

Nguyen, Thien Phu *(Institute of General Mechanics, RWTH Aachen University, Templergraben 64, 52062 Aachen, Germany; Automotive Safety and Assessment Engineering Research Center, the Sirindhorn International Thai-German Graduate School of Engineering, King Mongkut's University of Technology North Bangkok, 10800, Thailand)*
Navrath, Uwe *(Institute of General Mechanics, RWTH Aachen University, Templergraben 64, 52062 Aachen, Germany)*
Heider, Yousef *(Institute of General Mechanics, RWTH Aachen University, Templergraben 64, 52062 Aachen, Germany)*
Carmai, Julaluk *(Automotive Safety and Assessment Engineering Research Center, the Sirindhorn International Thai-German Graduate School of Engineering, King Mongkut's University of Technology North Bangkok, 10800, Thailand)*
Markert, Bernd *(Institute of General Mechanics, RWTH Aachen University, Templergraben 64, 52062 Aachen, Germany)* 16:20

Foam has a wide range of applications, and the study of its properties and behaviors and mechanical response has gained a lot of attention in recent years. To deepen the understanding of foam's behavior, the underlying research project proposes a new study to determining the deformation-dependent permeability of foam using a combination of CT scans and the

Lattice-Boltzmann method (LBM). Specifically, the three-dimensional mesoscopic structure of foam is reconstructed under nano CT at different compression level including uncompressed (0%), 10%, 30%, 50% and 70% of compression. The scanner software Avizo is used to extract the foam properties, where the foam specimen is modified to cubic sample being suitable for experiment. After the processed and exported data from CT scans, the Lattice Boltzmann method is applied to simulate single-phase fluid flow in the deformed porous domain subjected to step-wise displacement-controlled compression. The permeability at each corresponding deformation stages is characterized and determined by the LBM using the open-access Palabos software. In this work, the deformation-dependent intrinsic permeability properties are considered by applying a meso-macro hierarchic upscaling scheme. According to the CT scan outcomes, the compression level is inversely proportional to the porosity. The physical phenomenon is discussed in detail and the effect of image resolution on the permeability computation accuracy is investigated. The resulting permeability measures are to be compared with reference data from the literature. Furthermore, an upscaling approach from CT scan and LBM on the mesoscale to the numerical modeling on the macroscopic scale will be discussed. In this, the application artificial intelligence, as using supervised artificial neural networks, can be very helpful in bridging the scales.

Guaranteed lower bounds to effective stiffness in 3D

Pultarová, Ivana *(Czech Technical University in Prague, Czech Republic)*
Gaynutdinova, Liya *(Czech Technical University in Prague, Czech Republic)*
Ladecky, Martin *(Czech Technical University in Prague, Czech Republic; University of Freiburg, Germany)*
Zeman, Jan *(Czech Technical University in Prague, Czech Republic)*

16:40

We compute effective stiffness tensors of linear elasticity operators of three-dimensional heterogeneous problems. We consider a cuboid domain and solve a standard homogenization equation in its variational form using some finite element discretization. Due to the variational scheme, any obtained sufficiently accurate numerical solution yields and upper bound to the stiffness tensor in the sense that the difference between the numerical and exact matrices is positive semi-definite. In our presentation, we focus on computing a lower bound to the stiffness tensor, which may be of interest in some safety related problems. To this end the dual problem is formulated and discretized. Since the solution of the dual problem is computationally more demanding than the solution of the primal problem, we suggest a less accurate but rather cheap method to obtain an approximate solution of the dual problem. The method builds a special field gained from the primal solution and its projection to the space of the compatible dual fields. For discretization of the dual problem we use Bogner-Fox-Schmidt finite elements or of some second order piecewise polynomial finite elements.

Homogenization of plane ring mesh under static loading

Dries, Fabian Werner *(TU Dresden, Germany; Technische Hochschule Ingolstadt, Germany)* 17:00
Wallmersperger, Thomas *(TU Dresden, Germany)*
Kessler, Jörg *(Technische Hochschule Ingolstadt, Germany)*

Plane ring meshes can be produced in large dimensions for various applications, e.g. in architecture or protective systems. The numerical simulation of all individual rings of ring meshes is very costly, which is why methods to abstract the structure have been sought in the past. In this paper, a method for determining the strain parameters of ring meshes under in-plane tensile loads is presented.

For this purpose, methods of rigid body analysis and representative volume elements with periodic boundary conditions are used. Furthermore, the determined strain parameters of the ring mesh are applied to finite elements. Green-Lagrangian strain tensors are determined for several exemplary ring meshes under different load cases. The obtained parameters are transferred to finite disk elements and compared with practical experiments in static load cases under dead weight. The comparison of the deformations of the ring mesh between numerical simulations and experiments show a very good agreement.

Modelling of single layer carbon-based nanostructures with a Reissner-Mindlin shell element including rotational degrees of freedom through approximation of the exponential Cauchy-Born rule and homogenisation of the interatomic potentials

Ochs, Julian *(University of Kassel, Germany)* 17:20
Wackerfuß, Jens *(University of Kassel, Germany)*

Graphene is one of the thinnest possible structures. It consists of a single layer of carbon atoms and possesses unique mechanical properties. The carbon atoms form bonds to neighbouring atoms which can be described by interatomic potentials. A simulation of molecular mechanical processes can be done by employing the formalism of the finite element method to the interatomic potentials [1]. Since a graphene layer consists of many atoms, a numerical simulation can be inefficient. A more promising way is to formulate a continuum theory on the atomistic level and derive the finite element approximation. The linkage between the continuum and the atomistic lattice can be done through a multiscale approach based on the Cauchy-Born Rule. However, the application of the standard Cauchy-Born rule is limited to volumetric crystals. This limit can be overcome in two ways: the higher order Cauchy-Born rule [2], which uses the second-order deformation gradient, and the exponential Cauchy-Born rule [3,4,5], which uses an exponential map, based on the curvature of the surface. In the contributions of all the aforementioned publications, subdivision elements are used for the finite element approximation. These elements have several drawbacks. First is the mesh generation cumbersome and second are only translational degrees of freedom considered. In the presented approach both aspects should be improved through the use of a shell model based on the Reissner-Mindlin kinematics with rotational degrees of freedom. The exponential Cauchy-Born rule is used to link the shell to the atomistic lattice. The surface and deformation parameters can be derived through the base vectors of the shell element. The

presented element is therefore able to use several interatomic potentials. The element formulation is verified and tested on a full-scale atomistic simulation in aspects of computation time and accuracy.

[1] Wackerfuß, J.: Molecular mechanics in the context of the finite element method. IJNME, 2009, 77-7, S. 969-997.
[2] Guo, X.; Wang, J. B.; Zhang, H.W.: Mechanical properties of single-walled carbon nanotubes based on higher order Cauchy-Born rule. IJSS, 2006, 43-5, S. 1276-1290.
[3] Arroyo, M.; Belytschko, T.: An atomistic-based finite deformation membrane for single layer crystalline films. JMPS, 2002, 50-9, S. 1941-1977.
[4] Findeisen, C.; Wackerfuß, J.: A modified approximation of the exponential Cauchy-Born rule for arbitrary shell-like nanostructures. *PAMM*, 2014, 14-1, S. 565-566.
[5] Hollerer, S.; Celigoj, C.C.: Buckling analysis of carbon nanotubes by a mixed atomistic and continuum model. CM, 51, 2013: 765-789.

Finite Element approximation for a homogenized plate bending model

Smoch, Christoph *(University of Bonn, Germany)*
Rumpf, Martin *(University of Bonn, Germany)*
Simon, Stefan *(University of Bonn, Germany)*

17:40

The talk presents a heterogeneous multiscale method for the approximation of isometric deformations of a homogenized plate model derived by Hornung, Neukamm and Velcic as a Γ-limit from three-dimensional elasticity for the thickness and the size of the microstructure simultaneously tending to zero. Our approximation is based on the Discrete Kirchhoff Triangle for the macroscopic deformation and we prove the convergence of discrete minimizers to a continuous minimizer. Additionally, we present numerical results and compare them to experimental results for fine scale laminated paper.

S09: Laminar flows and transition

Organizer(s): **Brenner, Gunther** *(TU Clausthal)*
Thevenin, Dominique *(U Magdeburg)*

S09-01: Laminar flows and transition

Date: May 31, 2023 14:00-16:00
Room: CHE/183

Boundary layer transition delay via biomimetic fish-scale arrays

Muthuramalingam, Muthukumar *(City, University of London, United Kingdom)* 14:00
Puckert, Dominik *(Institut für Aerodynamik und Gasdynamik, Stuttgart, Germany)*
Rist, Ulrich *(Institut für Aerodynamik und Gasdynamik, Stuttgart, Germany)*
Bruecker, Christoph *(City, University of London, United Kingdom)*

Aquatic animals have developed effective strategies to reduce their body drag during evolution. The present work investigates the effect of fish-type skins with overlapping scales on the boundary layer transition. Arrays of biomimetic fish scales in typical overlapping arrangements are placed on a flat plate in a low-turbulence laminar water channel. Transition to turbulence is triggered by controlled excitation of Tollmien-Schlichting (TS) waves. It was found that the scaled surface generates regular streamwise streaks which act to attenuate the TS waves. The streaks produce a spanwise averaged flow with a steeper velocity gradient than the Blasius solution (reference: flat plate case). This leads to a smaller shape factor which is known to stabilize the boundary. As a consequence of the streaks, the TS waves reorganise already early in the linear phase into weak lambda vortices with a spanwise wavelength the same as the fish scale array. Because of the stabilizing effect of the smaller shape-factor of the boundary layer the weak -vortices decay in the downstream direction. This proposed mechanism follows similar arguments given for the simulation of transition delay due to finite amplitude streaks. In the experiments, the transition location was substantially delayed in the downstream direction by 55% with respect to the uncontrolled reference case. This corresponds to a theoretical drag reduction of about 27%. We thus found that fish scales can stabilize the laminar boundary layer and prevent it from early transition, reducing friction drag.

Thermo-electrohydrodynamic convection in differentially rotating spherical shell

Gaillard, Yann *(BTU Cottbus-Senftemberg, Germany)* 14:20
Szabo, Peter *(BTU Cottbus-Senftemberg, Germany)*
Egbers, Christoph *(BTU Cottbus-Senftemberg, Germany)*

Large-scale convection in planetary interiors or atmospheres is usually investigated experimentally by observation or by small scaled laboratory experiments that do not lose the overall physical meaning of the flow dynamics. One example of such experiment models is the AtmoFlow spherical shell project aimed to investigate planetary atmospheres in a small-scaled spherical shell with pole-ward cooling and equatorial heating. To extend to a wide variety of

real planets, the shells of the model can rotate in a solid body configuration and is similar to Earth-like planets. However, the experiment is built such that the shells are able to rotate differentially. The latter is more an approximation given in boundaries of supermassive celestial bodies such as Jupiter or the Sun. To provide a central force field that mimics planetary gravity, an electric potential is applied between both shells filled with a dielectric fluid sensitive to thermal and electrical forcing. To complement the experiment, numerical simulations are conducted to define a parameter space that may be of interest to explore similarities that can be observed in free space.

The present study consists of a numerical investigation using a solver coded with the OpenFOAM ecosystem and runs dimensionless to solve the incompressible continuity, momentum, energy, and electric equations. The forcing is given by two main parameters the electric Rayleigh number counting for thermal and electric forcing and the Taylor number counting for the rotational forcing. Both parameters provide a Rayleigh-Taylor space to classify the observed flow structures. This study presents results for the case where the spherical shells rotate differentially and can induce Taylor vorticities ranging from the equatorial region to the pole-ward region and vice versa.

In addition, the thermal and electrical forcing can induce convection cells similar to Bénard cells where plumes of hot fluid detach at the inner shell and propagate outward in a radial direction. The main objective of this study is to identify regimes of stable flow below the Rayleigh and Kepler line in combination with electric forces that can break the symmetry in unstable regimes or even to extend the symmetrical behavior of the flow. To analyze the flow patterns a spatial Fourier analysis is used in addition to statistical moments.

Experimental study of perturbation growth in a round laminar jet

Gareev, Linar *(Lomonosov Moscow State University, Russian Federation)*
Ashurov, Denis *(Lomonosov Moscow State University, Russian Federation)*
Ivanov, Oleg *(Lomonosov Moscow State University, Russian Federation)*
Vedeneev, Vasily *(Lomonosov Moscow State University, Russian Federation)*

14:40

Jet flows often find applications in various technical processes such as temperature control, mixing, spraying and etc. Along with wide usage in technology and manufacture, jet flows are the object of fundamental science interest. Thus, a proper understanding of laminar-turbulent transition in them is highly important.

In this experimental work, we study round laminar submerged jet flow of air and introduction of controlled excitations to it. We conduct all our experiments and calculations at Reynolds number of 5400, based on average velocity and jet initial diameter D = 0.12 m. The jet is formed by a special short device, so that the jet flow has low exit pulsation level, large laminar region length (not less than 5D) and big jet diameter. This unique device allows us to track the evolution of small perturbations far downstream.

The first part of this work is contributed to the modal perturbation growth mechanism. Thin metal rings were put into the jet at small distance from the orifice to amplify unstable eigen modes of the jet by oscillating at different frequencies. There are three inflection points in the considered velocity profile, which generate two branches of growing perturbations according

to the linear stability analysis. Therefore, we used rings of two different diameters. Experimental and theoretically predicted wavelengths, radial distributions of velocity pulsations and amplification curves of modal perturbations were compared and a good correspondence was found.

The more recent investigation has been devoted to the non-modal perturbation growth in the considered jet flow. This idea has come from near-wall flows, in which, apart from the growth of instability modes, the non-modal (algebraic) mechanism of linear growth plays an important role. In unbounded flows, including submerged jets, the theoretical analysis of non-modal growth mechanism started only in the last decade. In experiments this mechanism has not been identified yet.

In order to excite algebraic perturbation growth, we put special wavy structures (deflectors) into the jet, which provide a roller-like transverse motion. The features of the transition to turbulence caused by this non-modal growth were considered. Based on obtained experimental results, we definitely identify the non-modal "lift-up" growth mechanism of introduced disturbances. The development of perturbations qualitatively corresponds to the theoretically calculated optimal perturbations, which are a priori non-modal.

The classical unsteady boundary layer: a numerical study

Kaczvinszki, Markus *(TU Wien, Austria)*
Braun, Stefan *(TU Wien, Austria)*
15:00

The transition process from a laminar to turbulent flow near a solid wall (e.g. at the suction side of a slender airfoil) is still not fully understood. We focus on the early stage of the flow transition based on boundary layer (BL) theory, i.e. high Reynolds number asymptotic expansions, which reduce the Navier-Stokes equations into simplified forms. While steady solutions of the resulting classical BL equations and corresponding regulations based on viscous-inviscid interaction theory are studied quite extensively, there is only few information about the fully time-dependent scenario. Hence, we numerically study the classical unsteady BL and its breakdown structure, the Van Dommelen-Shen singularity, on the simplest example we can imagine, the incompressible planar fluid flow through a rectangular channel with suction. The depicted BL builds at the lower channel wall and follows initially a generic Blasius behavior, which gets temporally modulated through suction by means of a slot located at the upper wall. As usual, the main part of the flow is inviscid and governed by Laplace's equation. Remarkably, the wall slip velocity, or alternatively the pressure gradient imposed on the BL, can be calculated in closed form and we have full control of its temporal dependency through the variation of the applied suction strength. This specific flow configuration allows us to split off the initial Blasius solution and promises us high accuracy solutions of the remaining unsteady BL equation in the scaled stream function formulation. Chebyshev collocation is used in wall-normal direction, where the infinite domain is mapped onto [-1,1]. In contrary, we discretize the mainstream direction with a finite difference scheme of second order accuracy, which proofs to be more precise near the build-up of singularities. In order to trigger a dynamic breakdown of the unsteady BL equations, we increase the suction rate continuously from zero to a level slightly above the critical value (obtained from the steady

case). As a consequence, the system can not relax to a steady solution and instead blows up in finite time at some mainstream position. We try to resolve this process with high resolution and the final goal is to verify the inner structure (the 2D blow-up profile) of the Van Dommelen-Shen singularity and its role in flow separation and transition.

Extension of Squires Theorem for Spatial Instabilities - On New Linear 3D Sub-Critical Oblique Modes

Oberlack, Martin *(TU Darmstadt, Germany)*
Yalcin, Alparslan *(TU Darmstadt, Germany)*
Laux, Jonathan *(TU Darmstadt, Germany)*

15:20

In his fundamental theorem, Squire (1933) showed that for time-evolving perturbations, 2D instabilities occur at the smallest Reynolds number, which is usually called the critical Reynolds number. We recently showed that this is not necessarily so for spatially evolving 3D modes. For this we introduced both a complex streamwise and spanwise wavenumbers (see Turkac, 2019, Yalcin, 2022), which gives rise to oblique 3D modes. Such modes have a neutral stability line (NSL) in the x-z-plane, which is oblique to the main flow direction.

Extending Squires idea by invoking symmetry methods in parameter space we show that oblique 3D instabilities at a Reynolds number below the critical 2D Reynolds number may exist. Using a direct numerical simulation and based on the extended approach, it is indeed possible to detect corresponding modes e.g. for the plane Couette flow.

Other than for temporally evolving modes, however, for spatially evolving modes the additional condition of group velocity (GV) must be taken into account, which states that the GV has to propagate in the direction of the spatially increasing mode. In other words, for 3D instabilities the vector of the GV must thus point into the unstable region, i.e. cross the above mentioned NSL in the x-z-plane.

We have worked out the above extension of Squire's theory based on Lie symmetries and will present it at the meeting as well as further details on the direction of the GV for the case of Couette flow and/or the Asymptotic Suction Boundary layer.

S09-02: Laminar flows and transition

Date: June 1, 2023 16:00-19:00
Room: CHE/183

Experimental investigation of the laminar-turbulent transition in coiled tubes with PIV and LDA

Müller, Conrad *(Otto-von-Guericke University Magdeburg, Germany)* 16:00
Kováts, Péter *(Otto-von-Guericke University Magdeburg, Germany)*
Zähringer, Katharina *(Otto-von-Guericke University Magdeburg, Germany)*

Helically coiled tubes are widely used in process engineering and biochemistry, especially in micro-reactors, to increase heat and mass transfer. Due to its excellent radial mixing without axial backmixing, it enjoys great popularity for homogenisation of momentum, temperature and concentration fields. At moderate Reynolds numbers, flows in helical reactors form the characteristic Dean vortices, which are steady laminar vortices. With increasing flow velocities, more complex vortex structures can be found, which, however, show a strong dependency on the geometry and setup. These structures can be divided into the primary Dean vortices, secondary Lyne vortices, as well as temporary vortex structures. The first investigations concerning transition in coiled tubes were already carried out by Taylor or White in 1929. Until today, there have been several experimental and numerical attempts to describe transition using a critical Reynolds number as a function of the curvature ration δ = d/D. Although it seems obvious, that the critical Reynolds number is shifted to higher values compared to straight tubes, the results and correlation attempts drift widely apart.

The reason may be found in different experimental and numerical set-up and here especially the inflow conditions. The smallest changes in the geometry and setup of the reactors can induce strong changes in the vortex occurrence. Therefore, we propose here the findings of Particle Image Velocimetry measurements (PIV), that were carried out in a simple straight helix with 6 turns, as well as in a coiled flow inverter reactor, which provides a 90°-degree rotation of the flow direction after one turn. Three independent measurements of 1000 images per Reynolds number (Re = 500...2400) each were performed with adapted acquisition frequencies between 0.6 and 1.5 kHz. It is shown that velocity fluctuations in the cross-section of a helix reactor behave differently at different points of the cross-section. There are only a few fluctuations in the bottom of the cross-section, while the fluctuations at the top at the outside of the coil are very strong, due to the formation of secondary vortices. The transition to full turbulence is studied now in a specially conceived device, that aims to exclude all effects of the inflow conditions by using already a coiled inflow section. The results of first measurements with Laser Doppler Anemometry (LDA) of comparable points of interest and Reynolds numbers will also be presented.

How to find the perfect application pattern for adhesives

Flaig, Florian *(TU Braunschweig, Institute of Dynamics and Vibrations, Braunschweig, Germany)* 16:20
Fräger, Timo *(TU Braunschweig, Institute of Dynamics and Vibrations, Braunschweig, Germany)*
Kaufmann, Marvin *(Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Bremen, Germany)*
Vallée, Till *(Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Bremen, Germany)*
Fricke, Holger *(Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Bremen, Germany)*
Müller, Michael *(TU Braunschweig, Institute of Dynamics and Vibrations, Braunschweig, Germany)*

In recent years in many areas of industrial production, adhesive bonding has become increasingly important. For this process, not only the durability of the bonded joint is of interest, but also the safe and cost-effective production. An important question here is how the adhesive flows in the gap and how it must be applied to achieve the desired final distribution. Air pockets must be avoided and adhesive leakage should be reduced. To approach this question, we have used methods that have been firmly established for the calculation of friction gaps and have transferred them to the problem of simulating adhesive flows.

A first goal is to understand the adhesive flow even with complex application patterns. To reach this target, we have experimentally investigated the pressing of different application patterns and quantified them using various methods for comparison with the simulation. In doing so, we quantified the fluid flow velocities in addition to comparing the resulting forces. It turned out that the results agree very well even with complex application patterns where flow fronts meet, air bubbles are trapped and deflate again.

The subsequent goal is the identification of optimised application patterns. For this purpose, we have followed 3 methods, an inverse simulation, artificial neural networks and classical optimisation algorithms that are discussed in this paper.

For the inverse simulation we use the following approach. First, an inverse simulation is used to obtain an inspiration for the initial pattern, which in a second step is slightly adapted to derive an optimal application pattern. It turns out that many different targeted distributions, especially rectangles can be produced by applying a variation of a star-like shape.

A similar strategy was followed with the artificial neural networks. There we trained a network to generate an initial application pattern for given final distributions. This method produced very similar results to the inverse simulation. Here too, a variation of the star shape is always found for different desired final distributions.

The classical optimisation aims at creating a pattern that undergoes practical restrictions by representing applicable initial distributions. For this purpose, application beads are defined by coordinates that can be approached by the application robot and the corresponding coordinates are optimized. Here it becomes apparent that adhesive leakage is unavoidable in the case of sharp corners that need to be filled completely. Another variation of the star shape is found as the optimal pattern here.

Numerical simulation of wood-polymer composites in hyperbolic dies

Liese, Fabian *(University of Kassel, Germany)*
Wünsch, Olaf *(University of Kassel, Germany)* 16:40

Wood fiber reinforced polymers are mainly processed by extrusion. In this work, the material behavior of wood-polymer composites (WPC) is modeled and numerical simulations are used to investigate the flow behavior. Rheological investigations can be used to determine shear-thinning flow behavior, which is also often considered in the numerical simulation of WPC processing dies and is mainly influenced by the polymer matrix. Fiber-fiber interaction increases shear viscosity and yield point formation can be observed. Cross-sectional changes are necessary in extrusion dies, in which strain as well as shear plays a significant role. In order to experimentally investigate and model the behavior of WPC under strain, measurements are carried out on hyperbolic dies, in which a uniaxial strain state exists and from which the strain viscosity can be derived. The flow state in the hyperbolic die is essentially defined by the velocity boundary conditions at the wall. By introducing a lubricant into the die, wall slip is experimentally generated and investigated, which is verified by means of the numerical simulations.

SPH simulations of non-Darcian fluid flow in porous materials

Krach, David *(University of Stuttgart, Germany; Stuttgart Center for Simulation Science)*
Steeb, Holger *(University of Stuttgart, Germany; Stuttgart Center for Simulation Science)* 17:00

Fluid flow through porous materials play a critical role in many scientific disciplines, for example in geoscience or materials science, and in technical applications, for example filters or fuel cells. The flow conditions are influenced by various factors, such as the boundary conditions that affect the Reynolds number *Re* and flow regime, as well as the structure of the porous material, with its inherent permeability and tortuosity. These effective parameters of the material exhibit a dependency from *Re*. In order to compute the effective material parameters, Direct Numerical Simulations of the flow at the pore scale are performed. As input data we use representative samples of real materials with small to moderate porosities ($\varphi \leq 0.2$), whose internal structure has been determined with a μXRCT scaning device and has subsequently been binarized. Due to the size of the domain with up to 1000^3 voxels, efficient parallelized algorithms are required to compute the flow in *3*-D samples with representative properties. We are developing an fully-Lagrangian Smoothed Particle Hydrodynamics (SPH) simulation framework designed to solve the weakly compressible Navier-Stokes equations. The solver is implemented on top of the software framework HOOMD-Blue [1,2] since this allows for massively parallel CPU and GPU computations. We present an approach focusing on single-phase fluid flow through porous media from moderate to higher Re-numbers ($1 \leq Re \leq 1000$) aiming to show a smooth transition of effective properties from creeping flow (Darcy regime) to the weak inertia regime.

[1] J. A. Anderson, C. D. Lorenz, and A. Travesset. General purpose molecular dynamics simulations fully implemented on graphics processing units. Journal of Computational Physics, 227(10):5342-5359, 2008.

[2] J. Glaser, T. D. Nguyen, J. A. Anderson, P. Lui, F. Spiga, J. A. Millan, D. C. Morse, and S. C. Glotzer. Strong scaling of general-purpose molecular dynamics simulations on GPUs. Computer Physics Communications, 192:97-107, 2015.

Numerical investigation of a mixed convection flow over a heated horizontal plate

Babor, Lukas *(TU Wien, Austria)* 17:20

The present study is concerned with the laminar mixed convection flow over a heated horizontal plate of finite length at zero angle of attack. Two different types of outer boundary conditions are considered. In the first case, the plate is placed in a channel with an infinite extent in the downstream direction and a uniform inlet velocity at a finite upstream distance from the plate. In the second case, the plate is located in a semi-infinite space, where a zero vertical velocity is prescribed at a finite distance in front of the plate.

The numerical solution of the Navier-Stokes equations for a large Reynolds number Re = 20000 is computed with the Finite Element Method and compared to the boundary layer solutions of Müllner and Schneider [1] and Schneider [2], which are valid for a vanishing Prandtl number (inviscid flow) and a small Richardson number. Goal-oriented adaptive mesh refinement is employed in order to resolve the thin viscous sub-layer.

The numerical solution converges to the boundary layer solution when the Prandtl number is decreased. In the case of a plate inside a channel the agreement between the numerical and asymptotic solutions is better the larger the channel height because the effect of the viscous sub-layer on the outer flow diminishes. The hydrostatic pressure difference between the lower and the upper side of the plate together with the Kutta condition at the trailing edge induce a circulation with a global effect on the flow around the plate. For the plate inside a channel and higher Richardson numbers, this additional circulation flow leads to flow separation at the bottom side of the heated plate. For certain parameters, we find multiple solutions of the steady two-dimensional Navier-Stokes equations which differ by the size of the separation bubble.

References

[1] M. Müllner and W. Schneider, *Heat Mass Transf.* **46,** 1097-1110 (2010).

[2] W. Schneider, *Proc. 3rd Eur. Therm. Sci. Conf.,* 195-198 (2000)

Investigation of the heat transfer coefficient for a red clay brick

Tibaut, Jan *(Graz University of Technology, Austria)*
Schanz, Martin *(Graz University of Technology, Austria)*
Gfrerer, Michael *(Graz University of Technology, Austria)* 17:40

There is a need for the development of materials that can store heat. Heat energy is used in different ways, e.g., for house warming or production of electricity from solar power plants. However, to use the heat energy efficiently isolating materials are needed. There are different materials available to isolate houses and storage containers. However, those materials are expensive and some are over engineered. The best available material for isolation of heat would be air that has the thermal coefficient λ_{air}=0.02446W/mK. Thus, materials that trap a

large amount of air are good isolators. On the other hand, some isolating materials are harmful for the environment, e.g., glass wool, asbestos. An alternative are red clay bricks because red clay is a natural product that is present everywhere on the planet. But the thermal coefficient of red clay bricks is high λ_{brick}=0.6W/mK. To reduce the thermal coefficient cavities can be added in the brick. The cavities trap air and reduce the thermal coefficient of the brick. The heat transfer of a red clay brick can be numerically simulated. To determine the heat transfer coefficient of a red clay brick, heat transfer in form of conduction, convection and radiation is considered. The Boundary-Domain Integral Method (BDIM) was used to solve the natural convection of air in an enclosed cavity. The problem of the method is that the computational complexity is quadratic $O(M^2)$, where M is the number of unknowns in the domain. There are different methods available to reduce the complexity of the BDIM from quadratic to logarithmic $O(M \log M)$ or linear $O(M)$. For the simulation of fluid flow the non-dimensional velocity-vorticity formulation of the Navier-Stokes equations is applied. These equations are reformulated into the Yukawa equation by approximating the time derivative by finite differences. The corresponding BDIM has been accelerated with the H^2-methodology. Laminar fluid flow is present in the cavities. Thus, the Rayleigh number is below 10^6. The cavities are also heated by heat radiation of the surrounding walls. Numerical studies will be presented.

S10: Turbulence and reactive flows

Organizer(s): **Schmidt, Heiko** *(BTU Cottbus)*
Stein, Oliver *(U Stuttgart)*

S10-01: Turbulence and reactive flows

Date: May 30, 2023 13:30-16:10
Room: CHE/184

Map-based stochastic modeling of multiscale transfer processes in turbulent flows

Klein, Marten *(BTU Cottbus-Senftenberg, Germany)* 13:30

The detailed modeling of turbulent mixing has remained a numerical challenge for a number of applications, ranging from chemically reacting flows to noise prediction in technical flows, and encompassing convection on multiple scales in the geophysical context, among others. Complications arise from the dynamical complexity of turbulence that manifests itself by emergent small-scale flow features, scaling cascades, and intermittency due to prescribed forcings, boundary and initial conditions. In order to robustly predict, for example, the occurrence of catalytic reactions, generation of mixing noise, or the heat transfer across a layer of fluid, it is crucial to represent the physical redistribution processes in the flow with a proper account of participating time and length scales. This yields scale-locality and causality constraints that can usually only be fully addressed by direct numerical simulation (DNS) based on the discretized three-dimensional (3-D) Navier-Stokes equations, which is a very costly undertaking and limited to moderate or low turbulence intensities. In order to overcome the fundamental limitations of statistical turbulence models and numerical cost of DNS, so-called map-based stochastic turbulence models have been developed and increasingly applied to various mutiphysical flows over the last couple of decades. These models utilize one-dimensional (1-D) generalized Baker's maps in order to distinguish advective filamentation from molecular diffusion processes, resolving all relevant scales of the flow along a single physical coordinate. Baker's maps are probabilistically sampled with respect to size, location, and time of occurrence which introduces dynamical complexity into the bottom-up modeling approach. When the sampling is based on the evolving flow state, a self-contained reduced-order model with predictive capabilities for turbulent flows can be formulated. In the talk, I will summarize the map-based stochastic modeling strategy with an emphasize on the so-called One-Dimensional Turbulence (ODT) model. After that, I will discuss some recent advances in the field, demonstrating the applicability of the approach across flow configurations. I will address in more detail the flow physics representation by means of entrainment and passive scalar mixing in turbulent jets, as well as heat flux and wall shear stress fluctuations in heated channels and stably-stratified atmospheric boundary layers.

Impact of spatially varying magnetic fields on turbulent thermal convection

Bhattacharya, Shashwat *(Technische Universität Ilmenau, Germany)* 14:10
Boeck, Thomas *(Technische Universität Ilmenau, Germany)*
Krasnov, Dmitry *(Technische Universität Ilmenau, Germany)*
Schumacher, Jörg *(Technische Universität Ilmenau, Germany; Tandon School of Engineering, New York University, USA)*

We analyze the influence of fringing magnetic fields on turbulent thermal convection in a horizontally extended rectangular domain. The magnetic field is created in the gap between two semi-infinite planar magnetic poles. The convection layer is located near the edge of the gap. We employ direct numerical simulations in this setup for a fixed Rayleigh number ($Ra=10^5$) and small Prandtl number (Pr = 0.021), but vary the fringe-width by controlling the gap between the magnetic poles and the convection cell. The magnetic field generated by the magnets is strong enough to cease the flow in high magnetic flux region of the convection cell.

It is observed that as the local vertical magnetic field strength increases, the large scale structures become thinner and are aligned perpendicular to the longitudinal sidewalls. The local heat transport is determined as a function of the local Hartmann number based on the vertical component of the magnetic field. Using these results, we estimate the global heat and momentum transport. We show that the global heat transport decreases with increasing fringe-width for strong magnetic fields and decreases with increasing fringe-width for weak magnetic fields. The convective motion becomes confined to the vicinity of the sidewalls in the regions of large vertical magnetic fields. The amplitudes of these wall modes show a non-monotonic dependence on the fringe-width.

So far, previous study on wall-modes has been restricted to magnetoconvection with electrically insulated walls. However, in realistic situations, the walls do have a finite electrical conductivity. In the current work, we study, for the first time, the impact of the electrical conductivity of the top and bottom walls as well as the sidewalls on the wall modes. We observe that the wall modes tend to disappear as the electrical conductivity of the walls increases.

SGS modeling in lattice Boltzmann method for non-fully resolved turbulent flows

Polasanapalli, Sai Ravi Gupta *(Brandenburg university of technology Cottbus-Senftenberg, Germany; Indian Institute of Technology Madras, India)* 14:30
Klein, Marten *(Brandenburg university of technology Cottbus-Senftenberg, Germany)*
Schmidt, Heiko *(Brandenburg university of technology Cottbus-Senftenberg, Germany)*

Nowadays, the lattice Boltzmann Method (LBM) is used as an alternative to traditional Navier-Stokes-based solvers to simulate all kinds of fluid flow and heat transfer problems. LBM is based on the discretization of the Boltzmann equation and LBM is a kinetic theory-based method that describes the evolution of particle distribution functions in phase space. Originally, LBM was restricted to uniform Cartesian coordinate domains, which limited the applicability. However, combining finite-difference, finite-volume, and finite-element approaches with LBM eliminates the drawbacks associated with the grid and domain shape. Approaches of that kind are termed Off-Lattice Boltzmann Method (OLBM). The main advantage of off-lattice methods is the ability to handle complex geometries and boundaries more easily but it is

computationally expensive compared to the traditional LBM. It is still an active research area, and its merits and limitations in comparison to the traditional LBM are being investigated.

Similar to traditional Navier-Stokes solvers, turbulent flows can be simulated in the LBM framework using direct numerical simulation (DNS), Reynolds-averaged Navier-Stokes equation (RANS), and large-eddy simulation (LES) approaches, where LES captures large-scale fluctuations at affordable cost. The subgrid-scale (SGS) representation, however, remains a challenge resulting in modeling errors and limited applicability that is not related to LBM per se. In fact, the SGS treatment is traditionally accomplished by closure modeling of the unresolved turbulence scales based on prescribed physical relations with the resolved scales. It is hence not surprising that the accuracy of an LBM-LES can be significantly impacted by the choice of the SGS model in a given application. Therefore, it is important to select the right model for each application. Current research activities aim to make a leap in LBM-LES by utilizing stochastic turbulence models on the SGS scale, improving predictability and accuracy. In the present work, the implementation and assessment of different constant and self-adapting (i.e. dynamic) SGS models is performed as a first step utilizing the OLBM framework. The results obtained with traditional models provide benchmark cases, facilitating forthcoming research utilizing stochastic SGS modeling within OLBM for turbulent flows.

Spatio-temporal evolution and kinematic properties of large-scale coherent structures in fully developed turbulent pipe flow

Shahirpour, Amir *(Bayreuth University, Germany)*
Sesterhenn, Jörn *(Bayreuth University, Germany)*
14:50

Kinematic properties of large-scale coherent structures are investigated in fully developed turbulent pipe flow. Given the multi-scaled and complex nature of turbulent flows, it is of high interest to decompose the flow fields and study each set of structures identified by their length scales and group velocities. While traditional data-driven methods such as Proper Orthogonal Decomposition (POD) and Dynamic Mode Decomposition (DMD) can successfully reduce flows with stationary features, they fail to describe transport-dominated structures appearing in wall-bounded flows.

We resolve this issue by applying a Characteristic DMD (CDMD) (Sesterhenn and Shahirpour 2019) to time-resolved numerical data. In this approach the structures are followed in a properly chosen frame of reference along the characteristics of the flow which are also represented by the group velocities of the energetic structures. The latter takes place using a coordinate transformation from physical into spatio-temporal space. The transformation is in form of a rotation in space and time with the rotation angle corresponding to the most dominant group velocity in the flow, determined by the maximum drop of the singular values. The transformed snapshots are decomposed via the standard DMD algorithm.

A subset of the spatio-temporal modes is selected so that their reconstruction optimally represents the spectral peak in premultiplied energy spectra in physical space. The latter modes form a subspace which accommodates large-scale features of the flow. DMD spectrum, mode coefficients and kinetic energy of the modes are then used to detect further subspaces interacting with each other and with the coherent structures. The chosen subspaces are reconstructed in the spatio-temporal space and transformed back to physical space. We show that

each subspace accommodates structures with certain wavelengths and how they correspond to streamwise and azimuthal energy spectra. Each reconstruction represents a reduced order model of the flow and is analyzed in terms of their temporal evolution, life-times, oscillation frequencies, energy content and their contribution to Reynolds stress tensor.

Effects of Reynolds number on turbulent concentric coaxial pipe flow using stochastic modeling

Tsai, Pei-Yun *(BTU Cottbus-Senftenberg, Germany)* 15:10
Schmidt, Heiko *(BTU Cottbus-Senftenberg, Germany)*
Klein, Marten *(BTU Cottbus-Senftenberg, Germany)*

Coaxial pipe flows with turbulent transfers are widely used in numerous engineering applications, such as heat exchangers, industrial chimneys, or chemical reactors, which require accurate modeling of the radial transfer process. A literature survey reveals that turbulent transfer in concentric annuli has been studied experimentally [1] and numerically [2] for low Reynolds numbers from a fundamental point of view. These studies have revealed notable wall curvature effects, which pose a challenge for modeling, in particular when the viscous length scale is not much smaller than the wall-curvature radius. Concentric coaxial pipe flows with high Reynolds number and Prandtl number (Schmidt number) remain challenging for state-of-the-art numerical simulations and turbulence models due to resolution requirements or the need for non-universal wall-function modifications, respectively. Thus, a stochastic one-dimensional turbulence (ODT) model formulated for cylindrical geometry [3] is used here to address these challenges by previously demonstrated regime-spanning predictive capability [4, 5]. ODT is a dimensionally reduced flow model that can be economically utilized as a stand-alone tool. The ODT model aims to resolve all relevant turbulent flow scales by modeling the effects of turbulent eddies with a stochastically sampled sequence of mapping events punctuating the continuous (molecular-diffusive) flow evolution. In a preliminary study [5], the coaxial pipe flows coupled with momentum and passive scalar transfer investigating not-too-small radius ratios ($R_i/R_o > 0.1$) have been validated with reference data [6]. Still, a careful investigation of the flow's statistical features and scaling properties due to the presence of the inner cylinder wall has not been done. In the contribution, we will investigate the effects of the Reynolds number on pressure-driven turbulent concentric coaxial pipe flows reaching down to very small radius ratios ($R_i/R_o < 0.1$) relevant for electrostatic precipitators in gas cleaning [7].

References

[1] K. Rehme, *J. Fluid Mech.*, **64**:263, 1974.
[2] B. J. Boersma, W.-P. Breugem. *Flow Turbul. Combust.*, **86**:113, 2011.
[3] D. O. Lignell, V. B. Lansinger, J. A. Medina Mendez, M. Klein, A. R. Kerstein, H. Schmidt, M. Fistler, M. Oevermann, *Theor. Comput. Fluid Dyn.*, **32**:495, 2018.
[4] M. Klein, H. Schmidt, D. O. Lignell. *Int. J. Heat Fluid Flow,* **93**:108889, 2022.
[5] P.-Y. Tsai, H. Schmidt, M. Klein (2022). Accepted for publication by *PAMM*, Section 10.
[6] E. Bagheri, B.-C. Wang. *Phys. Fluids*, **33**(5):055131, 2021.
[7] J. A. Medina Méndez, C. Bacher, U. Riebel, H. Schmidt, *Eur. J. Mech. B*, 2022.

Large-eddy simulation of a channel flow over an irregular porous matrix

Sadowski, Wojciech *(Chair of Thermal Turbomachines and Aeroengines, Faculty of Mechanical Engineering, Ruhr-Universität Bochum, Bochum 44801, Germany)*
Sayyari, Mohammed *(Chair of Thermal Turbomachines and Aeroengines, Faculty of Mechanical Engineering, Ruhr-Universität Bochum, Bochum 44801, Germany)*
di Mare, Francesca *(Chair of Thermal Turbomachines and Aeroengines, Faculty of Mechanical Engineering, Ruhr-Universität Bochum, Bochum 44801, Germany)*
15:30

We investigate the influence of the irregularity of the porous structure on turbulent characteristics of a channel flow over a porous matrix. In the porous region, the expectation in literature is that the irregularity of the matrix would not affect the global parameters of turbulence, e.g., turbulent length scale and anisotropy. In the context of a channel flow over packed beds, however, the global parameters of the porous medium can influence the turbulent flow over the bed, dominated by the Kelvin-Helmholtz instability (large-scale flow features). We will investigate these effects numerically using large-eddy simulation and analyze turbulent characteristics in the channel and porous region using filtering operators. In addition to turbulent characteristics, the anisotropy of the stress components, and relevant length scales, we intend to study the mean velocity-drag force relation. We will examine the flow statistics based on two comparable setups—first, a regular three-dimensional porous matrix consisting of an array of cubes to establish reference. Then, we will randomly perturb the locations of the cubes from the regular arrangement, resulting in an irregular structure. We will compare the flow characteristics in both setups and establish the effects of irregularity. Given the precedence in literature, we will verify whether the irregularity of the matrix setup presented does not affect the pore-scale prevalence hypothesis, i.e., the size of the turbulent length scale is smaller than the pore size. On the other hand, we expect that the local magnitude of perturbations in the obstacle placement will have a global effect on permeability, affecting the drag force and influencing the Kelvin-Helmholtz instability.

S10-02: Turbulence and reactive flows

Date: May 31, 2023 14:00-16:00
Room: CHE/184

Infinite Lundgren hierarchy of turbulence: Isotropy, super-isotropy and a finite dimensional eigenvalue problem

Görtz, Simon *(TU Darmstadt, Germany)* 14:00
Conrad, Johannes Heinrich *(TU Darmstadt, Germany)*
Oberlack, Martin *(TU Darmstadt, Germany)*

Our modern understanding of turbulence is focused on its statistical behavior. We therefore analyze Lundgren's infinite but linear multi-point hierarchy of probability density functions (PDF), which emerges directly from the Navier Stokes equations. We consider the limit of homogeneous isotropic turbulence (HIT), for which we revisit an (quasi)exact solution of the LMN hierarchy. To account for the physical properties of HIT, we introduce spherical coordinates and obtain a dimensional reduction in the two-point case n = 2. We further extend the concept of isotropy for PDFs to higher order which naturally leads to super-isotropy. This leads to a further dimensional reduction, since each of the PDFs then only depends on time t, the spherical radius r, the radial sample space velocity component v_r and the absolute value of the sample space velocity components orthogonal to the radial component v_t. Since the resulting reduced super-isotropic PDF hierarchy is still linear, we formulate a superposed product ansatz for the PDF in the function $h_m=h_m(t,r,v_r,v_t;\lambda_m)$. The superposition of eigenfunctions with eigenvalues λ_m is necessary since it takes into account the statistical coupling of processes on different scales. For a solution to have the proper character of a probability density function, the Lundgren hierarchy comes with a number of side conditions. These conditions are consequently reduced for the case of super-isotropy. Applying the permutation condition greatly simplifies the hierarchy of equations, since it yields the same functional form for all h. With this simplification, the initially infinite dimensional hierarchy is reduced to a single but non-linear integro-differential equation. The resulting equation together with the associated side conditions forms an eigenvalue problem for the eigenvalues λ_m, since the eigenfunctions have to be superposed in order to fulfill all side and boundary conditions, such as PDF decaying to zero for $v \rightarrow \pm \infty$. We further give an outlook on approaches to obtain a solution. We state that the dimensionally reduced system admits additional symmetries, which allow further insight into new scaling laws and the underlying turbulence physics.

Random field modeling of turbulent flows in industrial production processes of non-woven textiles

Antoni, Markus *(University of Kassel, Germany)*
Kürpick, Quinten *(University of Kassel, Germany)*
Lindner, Felix *(University of Kassel, Germany)*
Marheineke, Nicole *(Trier University, Germany)*
Wegener, Raimund *(Fraunhofer ITWM, Germany)*

14:20

In this talk we present a novel random field model for the stochastic reconstruction of turbulent flows in the context of the k-epsilon model. Our approach allows for computationally inexpensive simulations and is based on specific transformation formulas for stochastic Fourier-type integrals in combination with a suitable multi-scale strategy. The model is motivated by an application concerning industrial production processes of non-woven textiles.

ODT augmented RaNS

Glawe, Christoph *(wpd Onshore GmbH & Co. KG, Germany)*
Klein, Marten *(Lehrstuhl Numerische Strömungs- und Gasdynamik, BTU Cottbus-Senftenberg)*
Schmidt, Heiko *(Lehrstuhl Numerische Strömungs- und Gasdynamik, BTU Cottbus-Senftenberg)*

14:40

On one hand stochastic 1D models like the One-Dimensional Turbulence model (ODT) [1] describe diffusive and turbulent terms on small spatial scales down to the Kolmogorov scale with high computational efficiency but are not applicable to a complex geometry. On the other hand Reynolds-averaged Navier-Stokes (RaNS) solutions describe complex boundary conditions but lag of statistical richness of the flow especially close to the wall. One-way coupling a ODT model with a RaNS solution allows to calculate meaningful statistical properties. For a steady RaNS solution this leads to an ODT enhanced dynamical post processing. Other coupled systems of ODT and 3D flows are described by the author [2, 3] and others [4, 5, 6]. We will present the concept of ODT enhanced postprocessing by calculating exemplary probability density functions (PDF) of wall shear stresses.

[1] Kerstein, A. R. and Ashurst, W. T. and Wunsch, S. and Nilsen, V. One-dimensional turbulence: Vector formulation and application to free shear flows.J. Fluid Mech. , (2001) 447: 85-109.
[2] Glawe, C. ODTLES: Turbulence modeling using a one-dimensional turbulence closed extended large eddy simulation approach. Ph.D. thesis, (2015).
[3] Glawe, C, Medina M., JA, Schmidt, H. IMEX based multi-scale time advancement in ODTLES. Z Angew Math Mech. (2018) 98: 1907- 1923.
[4] Schmidt, R. C., Kerstein, A. R., McDermott, R., ODTLES: A multi- scale model for 3D turbulent flow based on one-dimensional turbulence modeling. Comput. Methods Appl. Mech. Engrg. (2008) 199:865-880.
[5] Cao, S., Echekki, T. A low-dimensional stochastic closure model for combustion large-eddy simulation.J. Turbul (2008) 9:1-35.

[6] Sannan, S., Weydahl, T., Kerstein, A. R. Stochastic simulation of scalar mixing capturing unsteadiness and small-scale structure based on mean-flow properties. Flow Turbul. Combust. (2013) 90:189- 216.

Transition in the torque scaling in a very wide gap turbulent Taylor-Couette flow (η = 0.1)

Hamede, Mohammed Hussein *(Brandenburg University of Technology Cottbus - Senftenberg, Germany)*
Merbold, Sebastian *(Brandenburg University of Technology Cottbus - Senftenberg, Germany)*
Egbers, Christoph *(Brandenburg University of Technology Cottbus - Senftenberg, Germany)*

15:00

The flow between two concentric independently rotating cylinders is a famous model for studying turbulent shear flows. The so-called Taylor-Couette flows (TC) have a simple geometry, and it is defined by the radius ratio η = r1/r2, with r1 and r2 the inner and outer cylinders radii respectively, the gap width d = r2 $-$ r1, and the aspect ratio Γ = L/d, where L is the length of the system. The kinematics of the system is defined by the rotation ratio μ = ω2/ω1, with ω1 and ω2 being the inner and outer cylinder rotation velocities respectively. Further, the shear driving the flow is represented by the shear Reynolds number introduced by Dubrulle et al. (2005): Res = (2 r1 r2 d)|ω2 $-$ ω1|/(r1 + r2)ν, where ν is the fluid kinematic viscosity. In this study, we investigat the turbulent Taylor Couette flow in a very wide geometry η = 0.1, with a pure inner cylinder rotation and stationary outer cylinder μ = 0, for different ReS ranging from 5000 to 150000. The radial (ur) and the azimuthal (uφ) velocity components were measured at different heights using high-speed particle image velocimetry (Hs-PIV). From the measured velocities, the angular momentum transport (N uω) through the gap is calculated. For a critical value of shear Reynolds number Res,cr = 25000 a change in the scaling exponent occurs between the Nusselt number and the shear Reynold number, where for Res $\geq$ 25000, a scaling of N uω $\sim$ Re^0.76 s is found, where this change of scale is related to the transition from the classical turbulent regime (where the flow in the bulk is turbulent but laminar in the boundary layer) to the ultimate regime (both bulk and boundary layers are turbulent) (Merbold et al. (2013)).
Further, a spectral analysis is done for the different investigated cases, where the variation of the pre-multiplied azimuthal energy co-spectra with respect to different wave numbers is analyzed. The main observation was that in the classical regime, the energy achieves two peaks, one for small and the other for large-scale structures, and the amplitude of the small structures decreases as Res approaches Res,cr . While in the ultimate regime, only one peak for large-scale structure was observed

Anisotropy and relaminarisation of the turbulent flow near a rotating cylindrical cavity wall

Hultsch, Thomas *(TU Dresden, Germany)* 15:20
Rüdiger, Frank *(TU Dresden, Germany)*
Stiller, Jörg *(TU Dresden, Germany)*
Fröhlich, Jochen *(TU Dresden, Germany)*

Rotor internal cooling is a new concept for cooling high power density electric vehicle drives. A turbulent pipe flow enters a cylindrical cavity in the rotor with a larger radius, forming a jet. The flow is deflected in the cavity and exits through an annular duct formed by the stationary pipe wall on the inside and the rotor wall on the outside. The opposing effects of rotation on the turbulence are superimposed creating a complex transitional flow. The strong shear layers in the jet region cause high turbulence production. The centrifugal forces due to the flow rotation, on the other hand, reduce the turbulent fluctuations.

The spectral element solver Semtex [1] is used to simulate the flow. Semtex is capable of solving the incompressible Navier-Stokes equations in an axisymmetric domain using cylindrical coordinates. The domain is discretised with elements of polynomial order 10 in the meridional plane and a Fourier expansion in the circumferential direction. A third order semi-implicit scheme is used for time integration. To stabilise the solver and to account for the smallest turbulent eddies, a spectral vanishing viscosity approach is employed.

In the contribution, the flow and turbulence properties of two cases, one with and one without rotation of the cavity wall, will be compared in detail. The mechanisms of turbulence production and attenuation due to rotation affect different components of the Reynolds shear stress tensor. This results in highly anisotropic turbulence. In certain areas, where the turbulence attenuation is strongest, the flow even relaminarises. Since the cooling efficency depends on the turbulent heat transfer of the flow, the local turbulence characteristics are key quantities for the cooling application.

[1] Blackburn, H.M., Lee, D., Albrecht, T. and Singh, J.: Semtex: A spectral element-Fourier solver for the incompressible Navier-Stokes equations in cylindrical or Cartesian coordinates, Comput. Phys. Commun., 245, 106804 (2019).

Higher-order moments of three velocity components in pipe flow at high Reynolds number

Furuichi, Noriyuki *(National Institute of Advanced Industrial Science and Technology, Japan)* 15:40
Ono, Marie *(National Institute of Advanced Industrial Science and Technology, Japan)*
Tsuji, Yoshiyuki *(Nagoya Univ., Japan)*

In order to investigate universal structure of a wall-bounded turbulence, high Reynolds number experiments, which is not influenced by viscosity, is focused by many researchers in recently. In generally, as the Reynolds number increases, difficulty of the measurement such as a spatial resolution issue increases. Since there is no absolute indicator for the validity of experimental data, there is endless debate about the reliability of examined data set. Higher order moment is possible to use as one of the indicator to know the accuracy of the turbulence statistics. The check of a convergence of the higher order-moment gives clearly the validity of the probability density function. Additionally, with assuming that the probability density

function is accurately obtained, the higher-order moment can contribute to the consideration for the universal structure. Meneavue and Marusic (2013) found that the logarithmic behavior, which is expected from attached eddy hypothesis, is observed in the profile of the higher-order even moment. To that the logarithmic region emerges from lower to higher-order even moment, the probability density function in there must have self-similarity or universality although it has not been clarified well.

To this end, we measured the three velocity components in the pipe flow using LDV at high Reynolds number up to Re_t=20750. The experiments were conducted at Hi-Reff. The reliability of the experimental data is checked by the detail comparison with other experimental and numerical data regarding the mean profile and turbulence intensity profiles. Using data set obtained, we analyze the higher-order moment and its Reynolds number dependency. For the streamwise and spanwise components, the logarithmic regions emerge from 2nd to 10th order even moments at $0.055\ Re_\tau < y^+ < 0.25\ Re_\tau$. The observed region is narrower and the start position is farer from the wall than previous researches. On the other hand, the logarithmic behaviors with different slope are found at $2\ Re_\tau^{0.5} < y^+ < 0.055\ Re_\tau$ for both components. The Reynolds number dependences of the logarithmic slope are also different in both regions. For the wall-normal component, the turbulence intensity is constant according to the attached eddy hypothesis. In this experiment, the constant region is emerged clearly in higher-order even moment at $2\ Re_\tau^{0.5} < y^+ < 0.055\ Re_\tau$. The results obtained in this experiment clearly indicate that the logarithmic region has two different structures in terms of the turbulence statistics.

S10-03: Turbulence and reactive flows

Date: June 1, 2023 16:00-19:00
Room: CHE/184

Towards green energy from metal fuels: numerical methods for fluid flow, heat transfer, and many reacting particles

Scholtissek, Arne *(TU Darmstadt, Germany)* 16:00
Mich, Johannes *(TU Darmstadt, Germany)*
Nguyen, Bich-Diep *(TU Darmstadt, Germany)*
Braig, Daniel *(TU Darmstadt, Germany)*
Hasse, Christian *(TU Darmstadt, Germany)*

Metals can serve as carbon-free energy carriers, e. g. in innovative metal-metal oxide cycles as proposed by Bergthorson (Prog. Energy Combust. Sci., 2018). For this purpose, iron powder is a suitable candidate since it can be oxidized with air, exhibits a high energy density, is non-toxic, and abundant. A particularly promising scenario with relevance to the energy transition is the retrofit of phased-out coal power plants for operation with iron as a fuel. While a multitude of mathematical models and simulation approaches is already available for other solid fuels, such as coal and biomass, modeling the combustion of iron dust flames is novel in many ways. The present work attempts to give an overview of modeling approaches including the peculiar properties of the combustion of single iron microparticles, which can become temporally liquid during thermal overshoots and whose oxidation rate can be kinetically controlled or limited by oxygen diffusion through the particle boundary layer. Beyond the particle scale, reaction fronts in iron-air suspensions depend on the local flow regime, polydispersity and number density of the microparticle cloud, intraparticle heat and mass transfer, and radiation, all of which have to be captured by numerical models for predictive simulations. The variety of physical effects that need to be captured on multiple time and length scales make the combustion of metals a challenging, but also a very interesting research topic. After presenting the state of the art, future directions of research in this emerging topical area are briefly outlined.

Investigation dry reforming of methane over nickel using a one-dimensional model

Rakhi, Rakhi *(BTU Cottbus-Senftenberg, Germany)* 16:40
Günther, Vivien *(LOGE AB)*
Franken, Tim *(BTU Cottbus-Senftenberg, Germany)*
Mauss, Fabian *(BTU Cottbus-Senftenberg, Germany)*

In the field of catalysis, dry reforming, i.e., methane reforming with CO_2, is in the focus due to growing environmental concerns about oil depletion and global warning with a desire to produce synthesis gas. However, this process can lead to the formation of carbon which can cause catalyst deactivation, especially at industrial conditions. Nevertheless, the key to develop a more coke-resistant catalyst is a better comprehension of the reforming process at a molecular level. Regardless of all the investigations, the detailed path for the conversion of methane to syngas and carbon remains a controversial issue. Another problem in setting

up a reaction mechanism is the difficulty to define the thermodynamic data for intermediate surface species and this leads to the development of thermodynamic consistent surface reaction mechanisms in literature where the thermodynamic data is not used to calculate the rate coefficients of the reverse reactions. Rather the Arrhenius parameters for the forward as well as backward reactions are explicitly given in the reaction mechanism to establish thermodynamic equilibrium.

In this investigation, a kinetically consistent detailed surface reaction mechanism is developed which consists of 26 reversible reactions with the help of a one-dimensional model, LOGEcat. Our previous work constructs the basis of the present investigation. Further, a detailed sensitivity analysis of reversible reactions and reaction pathways is performed to understand the mechanism better. The mechanism is validated for dry reforming of methane over nickel catalyst, however, it can also be used for other processes, such as, steam reforming and partial oxidation. The mechanism is tested by comparing the simulation results with the literature experiments and simulations in a wide range of temperature. The new developed kinetically consistent surface reaction mechanism is able to accurately express the dry reforming of methane over the nickel catalyst for complete range of temperature and also provide a useful insight into the key rate determining steps.

Collision Dynamics of Particles and Bubbles in Gravity-Driven Flotation: A DNS Investigation

Tiedemann, Benedikt *(Technische Universität Dresden, Institute of Fluid Mechanics, Germany)* 17:00
Fröhlich, Jochen *(Technische Universität Dresden, Institute of Fluid Mechanics, Germany)*

One of the most important sub-processes in flotation is the particle-bubble encounter due to its direct impact on flotation recovery and the flotation rate constant. However, existing models for the prediction of collision events face major shortcomings. Existing analytical models show an inadequate estimation of particle-bubble collisions due to several simplified assumptions. Because of the complex flow structures and the intense mixing of particles and bubbles in flotation pulps, experimental studies were performed using simplified systems. Yet only few numerical studies able to capture the complexity of the flow-field were performed.
The contribution reports on initial results from direct numerical simulations to provide information on collision processes in flotation. Three-phase Direct Numerical Simulations with mono-sized air bubbles and mineral particles were performed. The continuous fluid phase is governed by the unsteady, three-dimensional Navier-Stokes equations for incompressible fluids discretized with a second-order finite-volume scheme on a staggered, Cartesian grid. Air bubbles are modelled as rigid spheres represented by their equations of motion and coupled to the fluid by an immersed boundary method. The solid particles are four-way coupled point particles governed by the sum of fluid and collision forces. A statistically homogenous flow is simulated using tri-periodic boundary conditions. All parameters were chosen to match real world conditions in mechanical flotation cells.
The main driver of particle and bubble movement in the conducted simulations is gravity. The

bubbles rise in the fluid, the mineral particles settle to the bottom. Turbulence is generated by bubble and particle movements. While the smallest investigated bubbles show a laminar recirculation zone, the recirculation zone of the largest bubbles is transitional. An increase in bubble and particle diameters leads to higher relative velocities between particles and bubbles and thus to an increase in the number of collisions. Further influences, parameters and statistics on particle-bubble, particle-particle and bubble-bubble encounter will be discussed the final contribution.

Numerical study on Turbulence-Chemistry-Interaction models for the partial oxidation of natural gas

Gonzalez Ortiz, Gabriel Alejandro *(Technische Universität Bergakademie Freiberg, Germany)* 17:20
Hutter, Martin *(Technische Universität Bergakademie Freiberg, Germany)*
Richter, Andreas *(Technische Universität Bergakademie Freiberg, Germany)*

The present work numerically investigates the application of two different turbulence-chemistry-interaction models, the standard Eddy Dissipation Concept (EDC) model and its extension the Partially Stirred Reactor (PaSR) model, for the partial oxidation of natural gas. For this, a comprehensive RANS model coupled with detailed chemistry is used to model both the fast oxidation reactions and the slow reforming reactions in ANSYS Fluent. The numerical results are validated against experimental data obtained from the semi-industrial high-pressure partial oxidation plant in Freiberg. The focus is to analyze the impact of the different reaction rate formulations on the flame characteristics and syngas composition. The PaSR model shows improvement over some known limitations of the EDC model, namely, the underprediction of the slow reforming reactions and the limitation of the length scale parameter at low turbulent Reynolds numbers. Additionally, a parameter study is carried out for the model constants.

Stochastic modeling of turbulent mixing based on a hierarchical swapping of fluid parcels

Starick, Tommy *(BTU Cottbus-Senftenberg, Germany)* 17:40
Schmidt, Heiko *(BTU Cottbus-Senftenberg, Germany)*

Turbulent mixing is an omnipresent phenomenon that constantly affects our everyday life. The mixing of two or more streams also plays an important role in a variety of chemical processes and industrial applications involving turbulent liquid or gaseous flows. The simulation of turbulent mixing poses great challenges, since the flow is often characterized by a wide range of length and time scales. A full resolution of all relevant length and time scales is associated with an immense computational effort and therefore not feasible for most engineering applications. This limitation can be overcome by means of a modeling of the sub-grid scales. Reynolds-averaged Navier-Stokes (RANS) and large-eddy simulation (LES) approaches are solving for an ensemble-averaged state and for a spatially-filtered ensemble-averaged state, respectively. However, in turbulent reacting flows, the accurate resolution of the sub-

grid scales is crucial because they involve reactive and diffusive transport processes. Transported probability density function (PDF) methods are widely used for the simulation of turbulent reactive flows because of the favorable treatment of the chemical source term. To capture the interaction in the sub-grid scales, transported PDF methods are using a molecular mixing model. The simplified modeling of the mixing is a known weak point. At this place, the Hierarchical Parcel-Swapping (HiPS) model developed by A.R. Kerstein [J. Stat. Phys. 153, 142-161 (2013)] represents a computationally efficient and scale-resolving turbulent mixing model. HiPS mimics the effects of turbulence on time-evolving, diffusive scalar fields. In HiPS, the diffusive scalar fields or a state space is interpreted as a binary tree structure, which is an alternative approach compared to the most common mixing models. Every level of the tree represents a specific length and time scale, which is based on turbulence inertial range scaling. The state variables are only located at the base of the tree and are treated as fluid parcels. The effects of turbulent advection are represented by stochastic swaps of sub-trees at rates determined by turbulent time scales associated with the sub-trees. The mixing only takes places between adjacent fluid parcels and is done at rates consistent with the prevailing diffusion time scales. In the talk, we will detail the HiPS mixing model, its formulation for variable Reynolds and Schmidt number flows, and then show results for the scalar energy spectra, the scalar dissipation rate, passive scalar PDF, and Richardson dispersion. These model investigations are an important step of HiPS for the application to more complex flow configurations.

Linear analysis of a turbulent swirl flame

Varillon, Grégoire *(Thermo-Fluid Dynamic Group, Technical University Munich, Germany)* 18:00
Kaise, Thomas Ludwig *(Laboratory for Flow Instabilities and Dynamics, Technical University Berlin, Germany)*
Oberleithner, Kilian *(Laboratory for Flow Instabilities and Dynamics, Technical University Berlin, Germany)*
Polifke, Wolfgang *(Thermo-Fluid Dynamic Group, Technical University Munich, Germany)*

Swirling jets are of practical interest in many industrial combustion systems, since the central recirculation region at the exit of the inlet provides an efficient way to anchor flames in a combustion chamber. However, swirling flows are also subject to inertial, or swirl, waves that provide a additional flow-flame feedback, hence an additional potential for unstable behaviour. In this work, we present a linear analysis of a reactive swirling jet carried out with the Linearized Reactive Flow (LRF) model [Meindl et al., Comb. Flame (2020)] applied to a turbulent flow. The LRF model is a holistic approach to tackle linear stability of realistic reactive flows. In that purpose, the LRF is extended to turbulent combustion model based on the triple decomposition [Hussain and Reynolds, J. Fluid Mech. (1970)]. Particular attention is drawn to the closure of the temporal mean and coherent fluctuation of the heat release rate. This framework enables the use of linear stability tools for realistic swirl flames. Based on this, we bring new insights on the propagation of swirl waves: their nature and speed. The

regions of high sensitivity of the flow are identified, paving the way to the control of swirl-induced instabilities. The conversion process of swirl waves to fluctuating heat release rate is finally studied in detail.

Assessing the Aeroacoustic Performance of the SSV-PANS Method for Slanted Back Ahmed Body

Moosavifard, Arezoo *(Technical University of Darmstadt, Germany)* 18:20
Schäfer, Michael *(Technical University of Darmstadt, Germany)*

The field of aeroacoustics examines the sound generated by the interaction between unsteady flows and solid structures, such as airplanes and cars. Research in this area can be conducted through theoretical, experimental, and computational methods. Computational Aeroacoustics (CAA), which uses computational fluid dynamics (CFD), has become a popular choice due to its ability to deliver acceptable results at a lower cost than experimental methods. The partially-Averaged Navier Stokes (PANS) method, a hybrid of Large-eddy Simulation (LES) and Reynolds-Averaged Navier-Stokes (RANS) techniques, is a well-established technique in CFD. The Scale-Supplying Variable (SSV) PANS method is a novel development within the PANS method that uses a modeled equation to compute resolved kinetic energy. It has been implemented in the in-house finite-volume solver FASTEST to compute the flows in complex applications. The SSV-PANS method is then applied to the incompressible flow field to calculate the aeroacoustic sources. The study aims to evaluate the aeroacoustic performance of the SSV-PANS method compared to a reference Large-eddy Simulation, focusing on accuracy and computation cost. A hybrid approach, which separates fluid variables into incompressible hydrodynamic and compressible perturbation equations, is used to study aerodynamic noise. The method is used to study the flow around the Ahmed Body, a well-established benchmark test case in Computational Fluid Dynamics (CFD), to study the performance of the SSV-PANS method in the context of aeroacoustics.

S11: Interfacial flows

Organizer(s): **Schwarzenberger, Karin** *(TU Dresden)*
Marschall, Holger *(TU Darmstadt)*

S11-01: Interfacial flows

Date: May 31, 2023 14:00-16:00
Room: CHE/S91

An arbitrary Lagrangian-Eulerian formulation for Navier-Stokes flow on deforming surfaces

Sauer, Roger A. *(Gdansk University of Technology, Poland; RWTH Aachen University, Germany; IIT Guwahati, India)* 14:00

A new arbitrary Lagrangian-Eulerian (ALE) formulation for incompressible Navier-Stokes flow on deforming surfaces is presented. The new formulation extends the surface ALE formulation of [1] to more general surface motions. It is based on a new curvilinear surface parameterization that describes the motion of the ALE frame. Its in-plane part becomes fully arbitrary, while its out-of-plane part follows the material motion of the surface. This allows for the description of flows on deforming surfaces using only surface meshes. The unknown fields are the fluid pressure, fluid velocity and surface motion, where the latter two share the same normal velocity. The new theory is implemented in the nonlinear finite element framework of [2] using the stabilization scheme of [3] for the incompressibility constraint. The implementation is verified through several manufactured steady and transient solutions, obtaining near optimal convergence rates in all cases. The new formulation allows for a detailed study of fluidic membranes such as soap films, bubbles and lipid bilayers.

[1] A. Sahu, Y.A.D. Omar, R.A. Sauer and K.K. Mandadapu (2020), Arbitrary Lagrangian-Eulerian finite element method for curved and deforming surfaces: I. General theory and application to fluid interfaces, J. Comput. Phys., 407:109253
[2] R.A. Sauer (2014), Stabilized finite element formulations for liquid membranes and their application to droplet contact, Int. J. Numer. Meth. Fluids, 75(7):519-545
[3] C.R. Dohrmann and P.B. Bochev, A stabilized finite element method for the Stokes problem based on polynomial pressure projections, Int. J. Numer. Methods Fluids, 46:183-201

A geometrical phase indicator for the unstructured finite-volume Level Set Method

Marić, Tomislav *(TU Darmstadt, Germany)*
Reitzel, Julian *(TU Darmstadt, Germany)*
Fricke, Mathis *(TU Darmstadt, Germany)*
Bothe, Dieter *(TU Darmstadt, Germany)*
Juric, Damir *(Laboratoire Interdisciplinaire des Sciences du Numérique CNRS, Orsay, France; Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK)*
Chergui, Jalel *(Department of Applied Mathematics and Theoretical Physics, University of Cambridge, UK)*
Shin, Seungwon *(Mechanical and System Design Engineering, Hongik University, Korea)*

14:20

Re-distancing commonly recovers the signed-distance property in the Level Set method for incompressible multiphase flows. The signed distance property is advantageous for phase indication and mean curvature calculation. However, re-distancing impacts volume conservation, contact line motion and overall accuracy. Instead of re-distancing, we propose a second-order geometrical phase-indicator approximation applicable to unstructured meshes with polyhedral cells. Using the geometrical approximation of the zero level set renders the signed-distance property unnecessary for the phase-indication, and provides a geometrical basis for alternative geometrical curvature and surface tension force approximations. There is a similarity in using the geometrical phase indicator in the Level Set method to the hybrid coupled Level Set / VOF method. However, we only borrow the geometrical phase indication from the VOF method. The proposed method demonstrates acceptable volume conservation, high phase-indicator advection accuracy, and high computational efficiency on unstructured meshes with arbitrary cell shapes.

Feedback stabilization of a surface tension system modeling the motion of a two-dimensional soap bubble

Court, Sebastien *(University of Innsbruck, Austria)*

14:40

Our aim is to design a feedback operator for stabilizing in infinite time horizon a system modeling the interactions between a viscous incompressible fluid and the deformation of a soap bubble. The latter is represented by an interface separating a 2-dimensional bounded domain into two connected parts filled with viscous incompressible fluids. The interface is a smooth perturbation of the 1-sphere, and the surrounding fluids satisfy the incompressible Stokes equations in time-dependent domains. The mean curvature of the surface defines a surface tension force which induces a jump of the normal trace of the Cauchy stress tensor. The response of the fluids is a velocity trace on the interface, governing the time evolution of the latter, via the equality of velocities. The data are assumed to be sufficiently small, in particular the initial perturbation, that is the initial shape of the soap bubble is close enough to a circle. Our approach relies on the approximate controllability of the linearized system. The latter is rewritten as an evolution equation dealing with the displacement of the soap bubble interface, involving in particular a Neumann-to-Dirichlet type operator. The control function

is a surface tension type force on the interface. We design it as the sum of two feedback operators: The first one is explicit, and the resulting operator defines an analytic semigroup of contraction, which implies that the unstable modes are now of finite number. The second operator is finite-dimensional, and is obtained as the solution of a Riccati equation. Both feedback operators are functions of the tangential derivatives of the displacement field. Their sum enables us to define a control operator that stabilizes locally the soap bubble to a circle with an arbitrary exponential decay rate, up to translations, and up to non-contact with the outer boundary. https://arxiv.org/abs/2205.15092

Monolithic Solver for Interfacial Flow Problems with Implicit Surface Tension

Afaq, Muhammad Aaqib *(TU Dortmund University, Germany)* 15:00
Fatima, Arooj *(TU Dortmund University, Germany)*
Turek, Stefan *(TU Dortmund University, Germany)*

We have developed a monolithic solver for interfacial flow problems which solves velocity, pressure and interface position simultaneously. The main idea of our work is based on the formulation discussed in [1,2], where it points out the feasibility of a fully implicit monolithic solver for multiphase flow problems via two approaches, a curvature-free level set approach and a curvature-free cut-off material function approach. Both formulations are fully implicit and have the advantages of requiring less regularity, since neither normals nor curvature are explicitly calculated. Moreover, the capillary time step restriction is eliminated, which is usually a big hindrance in performing the multiphase flow simulations with surface tension. Additionally, our robust solver is capable of performing the computations even for very large surface tension without destroying the interface. Furthermore, standard Navier-Stokes solvers might be used, which do not have to take into account inhomogeneous force terms due to surface tension. The reinitialization issue is integrated with a nonlinear term within the formulations. The nonlinearity is treated with a Newton-type solver with divided difference evaluation of the Jacobian matrices. The resulting linearized system inside of the outer Newton solver is a typical saddle point problem which is solved using a geometrical multigrid solver with Vanka-like smoother using the higher order stable FEM pair Q_2/P_1^{disc} for velocity and pressure and Q_2 for all other variables. The method is implemented into the FeatFlow [3] software package for the numerical simulation of multiphase flows. The robustness and accuracy of this solver is tested for different test cases, i.e. static bubble, oscillating bubble [4] and rising bubble benchmark [5], respectively.

[1] A. Ouazzi, S. Turek, and H. Damanik. A curvature-free multiphase flow solver via surface stress-based formulation. International Journal for Numerical Methods in Fluids, 88(1):18-31, 2018. https://doi.org/10.1002/fld.4509.
[2] E. Olsson, G. Kreiss, and S. Zahedi. A conservative level set method for two phase flow II. Journal of Computational Physics, 225(1):785-807, 2007.
[3] www.featflow.de. http://www.mathematik.tu-dortmund.de/featflow/en/index.html.
[4] M. A. Afaq, S. Turek, A. Ouazzi, and A. Fatima. Monolithic Newton-multigrid solver for multiphase flow problems with surface tension. In Book of Extended Abstracts of the 6th Eccomas Young Investigators Conference. Editorial Universitat Politecnica de Valencia, 2021. https://doi.org/10.4995./YIC2021.2021.12390.

[5] S. Hysing, S. Turek, D. Kuzmin, N. Parolini, E. Burman, S. Ganesan, and L. Tobiska. Quantitative benchmark computations of two-dimensional bubble dynamics. International Journal for Numerical Methods in Fluids, 60(11):1259-1288, 2009.

The effect of particles on the film drainage and bubble coalescence in a slurry bubble column

Liao, Yixiang *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)* 15:20

Understanding bubble coalescence in slurry columns and how it is affected by the presence of particles is of great significance to a variety of engineering applications. Despite decades of research, high-resolution data on the film drainage process in a bubble column are scarce, which prevents a precise description of the phenomenon and the derivation of reliable models for further analyses. The existing work on bubble coalescence in the presence of particles either focuses on experimental or analytical studies under nearly hydrostatic conditions with very low approach velocity (up to 0.1 mm/s), or is limited to a mesoscopic scale, for example, by acquiring void fraction and bubble size distribution changes in the column. The present work aims to fill the gap in-between and provide insights into the film drainage process at the microscopic scale under bubble column hydrodynamic conditions. By coupling the volume-of-fluid (VOF) and multiphase particle-in-cell (MP-PIC) methods with a chimera mesh approach in OpenFOAM, a high resolution of the interface and fluid flow field is realized and meaningful results on the effect of particles are achieved. In the investigated parameter range and condition, the presence of particles in the liquid is shown to affect majorly the film drainage process, while have negligible effects on the bubble rise and approach velocity. The influence of particle number concentration is found to be complex and multimodal in co-axial coalescence. At sufficiently low concentration, particles are pushed out from the film and do not alter the drainage and coalescence rate noticeably. As the concentration increases, first a physical blocking effect then a slight promotion because of the drainage changing from axisymmetry to asymmetry is observed. The drainage process is greatly retarded by a conjunct motion, where the bubbles rotate along the colliding interfaces. Furthermore, no dimple formation is observed at high concentrations, which is typical at low particle load or in pure liquids. As the film is thinned down to a critical thickness in the conjunct stage, the interface becomes wavy and instable leading to film rupture. The presence of particles captured in the thin film affects its stability greatly. Both particle size and density are shown to have a dual effect on the coalescence time. Increasing of them leads to first suppression then promotion of coalescence. The results on the effects of number concentration, particle size and density agree with the observations of the previous literature.

Eulerian simulations of premixed submerged multiphase turbulent jets: RANS based approach

Kamble, Vikrant Vinayak *(Technische Universität Dresden, Institute of Fluid Mechanics Helmholtzstrasse 10, Dresden, 01062, Germany; Helmholtz-Zentrum Dresden-Rossendorf, Institute of Fluid Dynamics, Bautzner Landstrasse, Dresden, 01328, Germany)* 15:40

Rzehak, Roland *(Helmholtz-Zentrum Dresden-Rossendorf, Institute of Fluid Dynamics, Bautzner Landstrasse, Dresden, 01328, Germany)*

Fröhlich, Jochen *(Technische Universität Dresden, Institute of Fluid Mechanics Helmholtzstrasse 10, Dresden, 01062, Germany)*

The recovery of mineral ores greatly depends on the hydrodynamics in a froth flotation process. Turbulent jets are created inside a froth flotation cell to enhance mixing, and thus improve recovery of mineral particles. Computational Fluid Dynamics (CFD) simulations provide a means to study such two- or three-phase turbulent jet flows by using mathematical models. The purpose of the current work is to validate the Euler-Euler CFD simulations in OpenFOAM using a set of interfacial closure models to predict the behavior of multiphase turbulent jet flows. Previously, simulations using this framework and validations were carried out for bubble columns by Rzehak and Kriebitzsch (2015) and for stirred tanks with solid-liquid flows by Shi and Rzehak (2020). The baseline closure models employed include drag, shear lift, virtual mass, wall forces, and turbulent dispersion forces for the gas-liquid as well as the solid-liquid interactions. In the present contribution, new CFD simulations using this framework are reported and validated with experimental results from Sun and Faeth (1986) for bubbly jets pointing in upward direction, and from Parthasarathy and Faeth (1987) for particulate jets pointing in downward direction. Along the axial and radial direction of the jet, a reasonable agreement is observed between the experimental and simulation results. Extending the scope of the topic, an attempt is made to simulate also three-phase premixed turbulent jets using the individually validated combination of closure models for both gas-liquid and solid-liquid jets jointly in the same simulations. Suitable data to validate the overall closure models for premixed gas-solid-liquid three-phase turbulent jet flows are not available in the literature. Thus, the simulations for three-phase turbulent jets are carried out in the same setup as used previously for the gas-liquid and the solid-liquid turbulent jets. A parametric study is carried out for the interfacial forces and an attempt to understand the interaction between the disperse and accompanying continuous phase will be presented.

Acknowledgements: This project has received funding from the European Union's Horizon 2020 Marie Skłodowska-Curie Actions (MSCA), Innovative Training Networks (ITN), and H2020-MSCA-ITN-2020 under grant agreement No. 955805.

References:

[1] Rzehak and Kriebitzsch, International Journal of Multiphase Flow 68, 135-152, (2015).

[2] Shi and Rzehak, Chemical Engineering Science 227, 115875 (2020).

[3] Sun and Faeth, International Journal of Multiphase Flow 12, 99-114, (1986).

[4] Parthasarathy and Faeth, International Journal of Multiphase Flow 13, 699-716, (1987).

S11-02: Interfacial flows

Date: June 1, 2023 08:30-10:30
Room: CHE/S91

Stability analysis of wall-attached Bénard-Marangoni convection in a vertical magnetic field

Boeck, Thomas *(TU Ilmenau, Germany)* 08:30

Thermal convection in a planar liquid layer with isothermal bottom and heat loss across the upper free surface appears as the result of a linear instability of the purely conducting state, to which both buoyancy and thermocapillary mechanism can contribute. We consider the Bénard-Marangoni instability where buoyancy is neglected, i.e. surface tension dependence on temperature is the cause of instability. An additional vertical magnetic field tends to suppress this instability when the liquid is electrically conducting. This effect was studied in the infinite layer model with horizontal periodicity. From the buoyancy-driven Rayleigh-Bénard convection it is known that convection is less suppressed by a magnetic field near electrically insulating side walls because induced eddy currents cannot flow unhindered near such a boundary. This effect is equally present in the Bénard-Marangoni instability problem and will be studied by a linear stability analysis of the purely heat-conducting state in a two-dimensional rectangular domain with side walls and a planar surface. In this analysis, periodicity is assumed in the third spatial direction. The heat transfer at the free surface is described by the usual single-layer approximation with a Robin-type thermal boundary condition and a Biot number. We also assume that the instability is of stationary type. The stability problem is solved by a spectral method using expansions in Chebyshev polynomials. The corner formed between the free surface and lateral boundary presents a difficulty that is circumvented by choosing simplified mechanical boundary conditions.

Bilayer Couette Flow over a Profiled Plate

Scholle, Markus *(Heilbronn University, Germany)*
Gaskell, Philip H. *(Durham University, UK)*
Ismail-Sutton, Sara *(Durham University, UK)*
Mellmann, Marcel *(Casculate, Kaiserslautern, Germany)* 08:50

We consider a shear-driven bilayer flow of two immiscible liquids between a planar and a corrugated plate under Stokes flow conditions, motivated by the use of fabricated surface texturing/topography as a means of enhanced friction and wear reduction and increased load carrying capacity in lubrication problems, partly inspired by biomimetic considerations. The starting point of the mathematical formulation is a variational principle which, in addition to the classical fluid mechanical field quantities, also includes potential fields, which in particular enables an elegant reformulation of the dynamic condition at the interface between the two layers. Two different methods of solution are utilised: (i) an analytic solution of the field equations, boundary and interface conditions is available by means of a long-wave approximation while (ii) an exact semi-analytic solution is obtained after transformation to complex variables by applying a spectral method. For validation purposes a numerical FE code based

on classical Navier-Stokes equations is implemented. Resulting streamline patterns, interface shapes and wall shear stresses are discussed.

Enhancement of interfacial instabilities by solid particles during fast stretching of a liquid suspension bridge

Brockmann, Philipp *(TU Darmstadt, Germany)*
Liu, Lu *(TU Darmstadt, Germany)*
Roisman, Ilia *(TU Darmstadt, Germany)*
Hussong, Jeanette *(TU Darmstadt, Germany)*

09:10

The liquid jet or liquid bridge stretching phenomenon is relevant to many industrial applications, such as atomization, crystallization, tire design, oil recovery, coating, and especially industrial printing processes.

During the stretching process, depending on the parameters, various phenomena such as finger instabilities, cavitation, and the formation and breakup of bridges have been observed. While these phenomena are the subject of numerous studies dealing with pure liquids, the effect of suspended particles is still unexplored. However, since solid particles are often present in liquids used in industrial processes, their influence on stretching dynamics is of great interest.

To investigate the effect of particles on the stretching dynamics of fluids and its stability, we have performed experiments with particle volume fractions ranging from 9.1% to 33.33% and particle sizes ranging from 13% to 88% of the original gap height.

We show that increasing particle volume fractions lead to increasing numbers of fingers during fingering instability. A comparison of the analytical results of Brulin et al. (2021) for pure liquids with our results indicates that this effect is due to the increased effective viscosity of the fluid caused by the particles and due to the initial interface disturbances of the interface.

Furthermore, we show that added particles also lead to the formation of secondary bridges in addition to the primary bridge when a certain ratio of initial gap height and droplet radius is exceeded. It is shown that as the volume fraction increases, the number of secondary bridges increases. Moreover, with increasing volume fraction, multiple bridges can be observed at lower ratios of initial gap height and droplet radius.

Non-invasive experiments of the fluid film behaviour in a horizontal rotating cylinder

Sommer, Oliver *(TU Chemnitz, Germany)*
la Monaca, Andrea *(University of Nottingham, UK)*
Bretschneider, Eric *(TU Chemnitz, Germany)*
Wozniak, Günter *(TU Chemnitz, Germany)*

09:30

Subject of our investigations is the spatial distribution of a Newtonian liquid within a partially filled horizontal rotating hollow cylinder in dependence of the variables angular velocity and angular acceleration, cylinder filling and cylinder geometry as well as viscosity of the liquid. We focus on the development of a thin liquid film at the inner cylinder wall which layer thickness was measured using a non-invasive laser-induced fluorescence measurement technique. In addition, the liquid distribution and flow topologies were observed and described

using optical measurements. The occurring liquid distributions can be distinguished in three different states. At low angular velocities most of the liquid is located at the bottom area of the cylinder. However, a thin liquid film is always pulled out of the reservoir from the rotating cylinder wall. With increasing angular velocity more and more liquid is deflected and the local measured film thickness increases. Exceeding a critical angular velocity, a centrifuged distribution of the whole liquid establishes. In this state the measured film thickness fits the theoretical calculated value quite well. Very complex liquid distributions and flow patterns develop in particular at the critical angular velocity. In detail, two critical angular velocities were verifiably, so-called transition points of liquid distribution. With deceleration of the system a second critical angular velocity exists. Below this value the centrifuged distribution of the liquid collapses and moves back again to the bottom of the cylinder. A thin film is still pulled out of this reservoir. The second critical angular velocity of the 'break down' is always smaller compared to the first critical angular velocity at which the centrifuged state develops. Both of them can be influenced using the investigated parameters. Eventually, we show that the locally measured film thickness depends on these parameters, too.

Extended Integral Boundary Layer method for reactive species mass transfer in rotating films

Kebinger, Simon *(Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria; cofinanced with CEST GmbH, Victor Kaplan Str. 2, A-2700 Wiener Neustadt (COMET program of the FFG, project number 865864))*
Brenn, Günter *(Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria)*
Steiner, Helfried *(Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria)*
09:50

Centrifugal force driven rotating films are often utilized for highly controlled, low liquid consumption wet processing of complex microscopic surface structures, as typically envisaged in semiconductor industry. Many studies in literature computationally investigated this flow in the limit of thin film approximation (TFA), solving the asymptotic equations with Pohlhausen-type integral boundary layer (IBL) methods. The elimination of the spatial dependence on the wall-normal coordinate makes the TFA-IBL concept an attractive alternative to the computationally far more expensive Computational Fluid Dynamics (CFD) approach, which would numerically solve a discretized representation of the full set of the governing equations including a further cost increasing two-phase model. The underlying boundary-layer flow assumption, however, still puts certain severe limitations to the scope of TFA-IBL, especially in the region near liquid jet impingement, and also on the posture of boundary conditions, which basically must be externally prescribed. The present work proposes a hybrid concept to overcome the latter limitation, particularly for species mass transfer with wall surface reaction. The proposed extended approach combines the TFA-IBL-based solution for the flow field with a Finite-Difference (FD) solution for the species transport, flexibly allowing for arbitrary wall surface reaction boundary conditions. The present concept has been tested for various surface reaction conditions and validated against CFD results as well as solutions from standard

non-extended TFA-IBL, when applicable to the chosen setting. The generally observed good agreement proved the proposed extended TFA-IBL as a robust, reliable, and computationally still very efficient approach for analysing in much detail and possibly further optimizing the film-based wet chemistry processing of microstructures.

Mass and momentum transport in vertically impinging jets on moving substrates at high Schmidt number

Kebinger, Simon *(Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria; cofinanced with CEST GmbH, Victor Kaplan Str. 2, A-2700 Wiener Neustadt (COMET program of the FFG, project number 865864))*
Brenn, Günter *(Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria)*
Steiner, Helfried *(Institute of Fluid Mechanics and Heat Transfer, Graz University of Technology, Austria)*

10:10

The present work computationally investigates the complex liquid flow field around a jet impinging vertically on a pre-wetted linearly moving substrate. Species mass transfer is considered as well, assuming a high-Schmidt number operating liquid and infinitely fast wall surface reaction, as frequently met in industrial surface wet processing applications. The investigation is based on extensive three-dimensional CFD simulations using the volume of fluid method as the two-phase flow model. The study focuses in particular on the effect of the thickness of the oncoming film, alternatively prescribed as δpref=20 μm, 40 μm, and 80 μm, on the momentum and mass transfer across the moving substrate. In the highly sheared region between the impingement point and the bow wave upstream, the mean level of wall shear stress is significantly increased for the lower pre-film thicknesses. The shape and the mean position of the bow wave, which was also characterized based on the local variation of the wall shear stress, only slightly changed. The observed significant increase in wall shear stress is not reflected by the wall mass fluxes, as indicated by only marginal differences in the Sherwood number beneath the bow wave for the different pre-film heights. Opposed to the trend of the shear stress, the Sherwood number is even lowest here for the smallest pre-film height, which also conflicts with the theoretically expected cubic-root dependence on shear rate, as suggested by classical boundary layer analysis. Downstream of the impingement, the vertical jet momentum, being redirected against the moving wall-normal direction, most efficiently counteracts the further growth of the concentration boundary layer for the smallest pre-film height, producing the relatively highest Sherwood number. The presently observed very different response of the mass and momentum transfer to the variation of the oncoming pre-film thickness basically does not comply with the generally assumed strong coupling between both transport processes. Measurements from suitably designed impinging jet flow experiments will provide further empirical evidence on this counterintuitive behaviour.

S11-03: Interfacial flows

Date: June 1, 2023 16:00-19:00
Room: CHE/S91

Moving contact lines for sliding droplets

Peschka, Dirk *(Weierstraß-Institut für Angewandte Analysis und Stochastik, Germany)* 16:00

In this two-part talk, some recent theoretical results on interfacial flows are presented and exemplified for sliding droplets. In the first part, the role of Navier slip and dynamic contact angle for interfacial flows with moving interfaces and contact lines will be discussed. While the role of Navier slip is now accepted and undisputed, similar laws for the dynamic contact angle are still debated. Following the work of Ren and E, I will present a simple model for moving contact lines and possible extensions, and discuss the implications for droplet flows on solid substrates. In the second part of the talk, I will report on ongoing work on wetting of soft (viscoelastic) substrates by liquid droplets and discuss some phenomena. Pierre-Gilles de Gennes called liquid substrates the ëpitome of perfection.Ïn this part of the talk, we will explore to what extent this statement might be true and what new phenomena are relevant for viscoelastic substrates. In particular, for polymeric or gel-like substrates, simple viscoelasticity may be insufficient to adequately describe the rich structure of the relevant nonlinear diffusion and phase separation processes. This presentation presents joint work with the authors of the manuscripts below and is based on current work in the SPP 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Surfaces*.

[1] Giacomelli, L., Gnann, M. V., & Peschka, D. (2023). Droplet motion with contact-line friction: long-time asymptotics in complete wetting. arXiv preprint `https://arxiv.org/abs/2302.03005`.

[2] Schmeller, L., & Peschka, D. (2023). *Sharp-interface limits of Cahn-Hilliard models and mechanics with moving contact lines*. arXiv preprint `https://arxiv.org/abs/2301.04968`.

[3] Giri, A. K., Malgaretti, P., Peschka, D., & Sega, M. (2022). *Resolving the microscopic hydrodynamics at the moving contact line*. Physical Review Fluids, 7(10), L102001.

[4] Peschka, D., Haefner, S., Marquant, L., Jacobs, K., Münch, A., & Wagner, B. (2019). *Signatures of slip in dewetting polymer films*. Proceedings of the National Academy of Sciences, 116(19), 9275-9284. [5] Wagner, B., Bommer, S., Peschka, D., Jachalski, S., & Seemann, R. (2018). *Impact of energy dissipation on interface shapes and on rates for dewetting from liquid substrates*. Scientific Reports, 8(1), 13295.

Interfacial effects at gas bubbles growing on microelectrodes

Han, Yifan *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)* 16:40
Bashkatov, Aleksandr *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; Twente University, The Netherlands)*
Babich, Alexander *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Huang, Mengyuan *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Yang, Xuegeng *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Eckert, Kerstin *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Mutschke, Gerd *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*

Gas evolution at electrolysis processes is a complex process which besides phase change involves flow and temperature phenomena, transport of species, and also electric effects due to charge distribution and the field applied. At microelectrodes, thermocapillary and Coulomb forces caused by local heating, charge adsorption at the interface, and surfactants are known to affect the bubble dynamics [1,2,3]. However, a recent analysis of experimental data revealed that the tracer particles used for measuring the interfacial velocity themselves influence the bubble dynamics. The current work studies to what extent the influence of the tracer particles can be understood as acting as a surfactant. It presents a corresponding numerical model to verify how different bulk concentrations of particles affect the bubble dynamics. Special attention is drawn to the interfacial velocity profile driven by capillary effects in order to match the simulation results with experimental data. Besides, the force balance of the bubble close to departure is analyzed to conclude the distribution of surface charge density.

[1] A. Bashkatov, S.S. Hossain, G. Mutschke, X. Yang, H. Rox, I.M. Weidinger, K. Eckert; On the Growth Regimes of Hydrogen Bubbles at Microelectrodes, Phys. Chem. Chem. Phys. 24 (2022) 26738.
[2] S.S. Hossain, A. Bashkatov, X. Yang, G. Mutschke, K. Eckert; Force balance of hydrogen bubbles growing and oscillating on a microelectrode; Phys. Rev. E 106 (2022) 035105.
[3] A.M. Meulenbroek, A.W. Vreman, N.G. Deen; Competing Marangoni effects form a stagnant cap on the interface of a hydrogen bubble attached to a microelectrode; Electrochim. Acta 385 (2021) 138298.

Hydrogen bubble motion reversals during water electrolysis

Babich, Alexander *(HZDR, Germany)* 17:00
Bashkatov, Aleksandr *(HZDR, Germany)*
Hossain, Syed Sahil *(HZDR, Germany)*
Yang, Xuegeng *(HZDR, Germany; Technische Universität Dresden)*
Mutschke, Gerd *(HZDR, Germany)*
Eckert, Kerstin *(HZDR, Germany; Technische Universität Dresden)*

The dynamics of hydrogen bubbles produced by water electrolysis in an acidic electrolyte are studied using electrochemical and optical methods. A defined cyclic modulation of the electric potential is applied at a microelectrode to produce pairs of interacting hydrogen bubbles in a controlled manner. Three scenarios of interactions are identified and systematically studied. The most prominent one consists of a sudden reversal in the motion of the first detached bubble, its return to the electrode, and finally its coalescence with the second bubble.

Attested by Toepler's schlieren technique, an explanation of contactless motion reversal is provided by the competition between buoyancy and thermocapillary effects.

Experimental investigation of Taylor bubble shape in narrow tubes with constrictions

Maestri, Rhandrey *(Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden)* 17:20

Bürkle, Florian *(Technische Universität Dresden, Fakultät Elektrotechnik und Informationstechnik, Professur für Mess- und Sensorsystemtechnik, Helmholtzstraße 18, 01062 Dresden)*
Büttner, Lars *(Technische Universität Dresden, Fakultät Elektrotechnik und Informationstechnik, Professur für Mess- und Sensorsystemtechnik, Helmholtzstraße 18, 01062 Dresden)*
Czarske, Jürgen *(Technische Universität Dresden, Fakultät Elektrotechnik und Informationstechnik, Professur für Mess- und Sensorsystemtechnik, Helmholtzstraße 18, 01062 Dresden)*
Hampel, Uwe *(Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden; Technische Universität Dresden, Fakultät Maschinenwesen, Professur für Bildgebende Messverfahren für die Energie- und Verfahrenstechnik, George-Bähr-Straße 3b, 01069 Dresden)*
Lecrivain, Grégory *(Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstraße 400, 01328 Dresden)*

Gas Taylor bubbles in millichannels are characterized by an elongated shape, bullet-shaped bubbles nose and a comparatively flat bottom. Because of dominant interfacial tension forces, such bubbles occupy most of the cross-sectional area of the tube. There exist many experimental or numerical investigations. Most of them consider Taylor bubbles moving in a straight pipe with constant cross-section, such as a tube or square duct. In this work, we report a new finding for a vertical tube equipped with a geometrical singularity. The dynamics of an individual Taylor bubble in a counter-current flow is presently investigated. We find that a small tube constriction, with only 5 % obstruction, has a significant influence on the flow and interfacial dynamics. Various regimes, characterized for increasing channel obstruction, are here established. High experimental and numerical reproducibility is observed.

Mapping the gas fraction distribution in bubble flows through open-porous foams by radiographic imaging

Lappan, Tobias *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden)* 17:40
Jiao, Guanghao *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden; Institute of Process Engineering and Environmental Technology, Technische Universität Dresden, 01062 Dresden, Germany)*
Michak, Robin *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden; Institute of Process Engineering and Environmental Technology, Technische Universität Dresden, 01062 Dresden, Germany)*
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Shevchenko, Natalia *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden)*
Trtik, Pavel *(Laboratory for Neutron Scattering and Imaging, Paul Scherrer Institut, Forschungsstr. 111, 5232 Villigen PSI, Switzerland)*
Eckert, Kerstin *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden; Institute of Process Engineering and Environmental Technology, Technische Universität Dresden, 01062 Dresden, Germany)*
Eckert, Sven *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf, Bautzner Landstr. 400, 01328 Dresden)*

The cost-efficient production of green hydrogen using renewable energies requires next-generation proton exchange membrane (PEM) electrolysers to be operated at higher current density. Under this new operating condition, the elevated temperature of the ultra-pure water and its supersaturation with oxygen on the anode side have strong effects on the formation and transport of gas bubbles. The resulting gas-liquid two-phase flow through the porous transport layer at the membrane electrode assembly is characterised by up to 50 % gas fraction, which is exceptionally high. Such a foam-like flow within the porous medium is not accessible by optical measurements. Instead, we performed imaging flow measurements by means of time-resolved radiography using polychromatic X-rays as well as thermal neutrons at 100 frames per second imaging frame rate. On a laboratory scale, we aimed to study the bubble transport by mapping the local gas fraction distribution over time. This conference contribution presents two model experiments with open-porous metal and polymer foams, namely made of nickel and polyurethane, showcasing the advantages but also limitations of X-ray and neutron radiography for investigating bubble transport phenomena within such foam structures. In both experiments, foam samples of approximately 70 mm x 70 mm in width and height were sandwiched between the X-ray- or neutron-transparent front and back windows of a vessel filled with deionised water. As neutrons are strongly attenuated by water, the thickness of the water-filled vessel and the foam sample were set to 5 mm along the beam direction in all measurements. Bubbles were generated continuously by injecting compressed air at different but constant volumetric flow rates through a single hollow needle releasing the bubbles directly into the water-soaked foam. Based on calibration radiographs acquired both in the absence and presence of water, quantitative image analysis yielded a

pixelwise mapping of the gas fraction at approximately 0.06 mm image pixel size without binning. While X-ray radiography visualised the pulsating transport of bubble plumes through a nickel foam of 1.2 mm pore size, neutron radiography gave insights into the jumping motion of single bubbles through a polyurethane foam of approximately 3 mm pore size. In conclusion, we characterised the gas transport depending on the volumetric gas flow rate, the bubble size in relation to the foam pore size and the wettability of the inner foam surface. Further radiographic studies will consider bubble flows through open-porous materials with different pore geometry or functionalised surface wettability.

Bubble generation by a plunging jet in the column of a pressurised pneumatic flotation cell

Zürner, Till *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Ortmann, Kilian *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Eckert, Kerstin *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; Technische Universität Dresden, Germany)*

18:00

The separation of minerals from inert stone by the froth flotation process has been used for over a century in the mining industry and a large fraction of today's ores is processed this way. By grinding the material into small pieces, the mineral particles are liberated. They are suspended in water and made hydrophobic, which has them attach to air bubbles and float to the top of the flotation cell. To increase the efficiency of extracting fine and ultra-fine particles (below 20 µm), stronger turbulence and smaller bubble sizes are advantageous.

Unlike conventional flotation, pneumatic flotation generates bubbles in a vertical column by impinging a particle-laden liquid jet on a free liquid surface and entraining the surrounding air. The air can be either drawn automatically or it can be supplied under pressure. The air flow is thus a new process parameter, which in self-aspirated flotation cells is not controlled directly as opposed to pressurised cells.

The bubble generation of a pressurised plunging water jet is studied in a laboratory scale model experiment. Control parameters are the water and air flow rate, as well as the concentration of added surfactant (MIBC). Measurements are performed by shadowgraphy imaging, pressure transducers and an electrical conductivity sensor. Results of interest are the distribution of the bubble size and gas volume fraction in the column.

Investigation of microalgae and bubble interaction in electroflotation via image processing

Marquardt, Tine *(Helmholtz-Zentrum Dresden-Rossendorf, Germany)*
Schwarzenberger, Karin *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; Technische Universität Dresden, Germany)*
Krujatz, Felix *(Technische Universität Dresden, Germany)*
Eckert, Kerstin *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; Technische Universität Dresden, Germany)*

18:20

Microalgae are becoming increasingly important for numerous applications such as food or pharmaceutical products. Flotation is an effective and comparatively inexpensive process for dewatering of the algal biomass after cultivation. In electroflotation, the hydrophobic algal cells attach to the surface of rising gas bubbles generated by water electrolysis and can

be removed as a concentrated froth. For enhanced floatability, the size of microalgae can be increased by flocculation, e.g., with chitosan. Chitosan is a non-toxic, non-contaminating biopolymer that has proven to be a practical flocculant for microalgae. The effectiveness of the flotation process is influenced by numerous variables. At the same time, the mechanisms of the attachment of the algae to the bubbles are not fully understood. Hence, the aim of the presented work is to gain a deeper insight into the processes involved in the electroflotation of microalgae, like the algae-bubble-interaction, using optical measurement methods and machine learning (ML) based image processing.

A main focus is on the number and size of bubbles generated by electrolysis, as well as the size of *Chlorella vulgaris* agglomerates created by flocculation with chitosan. The properties of the bubbles were influenced by changing the electrolysis voltage and evaluated by image processing methods on microscopic images. Using laser diffraction spectroscopy, the influence of different chitosan dosages and flocculation times on the agglomerate size were analyzed. The size distribution is found to depend strongly on the varying biological properties of the microalgal suspension. Nevertheless, some general recommendations for an optimal chitosan concentration range could be deduced. In order to identify conditions promoting a successful attachment of algae to bubbles, an ML based method using series of microscopic images for visualization of the rising bubble and agglomerate paths during bubble-algal interaction was developed. The results show that a similar size of bubble and microalgal agglomerate is beneficial for enhanced bubble-algae interaction. For the analyzed voltage range, the mean bubble size was approximately 20 µm. The flocculation experiments showed that agglomerate sizes of 20 µm or higher are also achievable and thus, the microalgae flocs can be tuned to a well-floatable size range. Summing up, it was possible to derive first conclusions on how to promote effective electroflotation of microalgae. The developed visualization method contributes to a better understanding of flotation mechanisms and can be used as a basis for further research.

Response of a surfactant- and particle-laden bubble surface to asymmetric shear flow

Eftekhari, Milad *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; TU Dresden)*
Schwarzenberger, Karin *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; TU Dresden)*
Heitkam, Sascha *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; TU Dresden)*
Javadi, Aliyar *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; TU Dresden)*
Eckert, Kerstin *(Helmholtz-Zentrum Dresden-Rossendorf, Germany; TU Dresden)*

18:40

The shear stress of an axisymmetric flow field triggers a nonuniform distribution of adsorbed surfactants at the surface of a rising bubble. This creates a surface tension gradient that counteracts the viscous shear stress of the flow and thus reduces the mobility of the interface. However, in technological processes the flow field often is asymmetric, e.g. due to the vorticity in the flow. Under such conditions, the interface experiences an unbalanced shear stress that is not free of curl, i.e. it cannot be compensated by the redistribution of the surfactants at the interface (Vlahovska et al., 2009). Here, we conduct model experiments with a bubble at the tip of a capillary placed in a defined asymmetric flow field, in the presence of

surfactants and nanoparticles. Unlike classical surfactants, nanoparticles adsorb irreversibly at the bubble surface. Thus, a different interaction between the bulk flow and the interface is expected. In this study, we show a direct experimental observation of the circulating flow at the interface under asymmetric shear stress (Eftekhari et al., 2021a,b). The results indicate that the interface remains mobile regardless of the surfactant concentration. Additionally, we show that the nanoparticle-laden interface adopts a solid-like state and resists the interfacial flow upon surface compression. Our results imply that the immobilization of the interface can be described by the ratio of the interfacial elasticity to the bulk viscous forces.

Vlahovska, P. M., Bławzdziewicz, J., & Loewenberg, M. (2009). Small-deformation theory for a surfactant-covered drop in linear flows. J.Fluid Mech., 624, 293.

Eftekhari, M., Schwarzenberger, K., Heitkam, S., & Eckert, K. (2021). Interfacial flow of a surfactant-laden interface under asymmetric shear flow. J. Colloid Interface Sci., 599, 837.

Eftekhari, M., Schwarzenberger, K., Heitkam, S., Javadi, A., Bashkatov, A., Ata, S., & Eckert, K. (2021). Interfacial behavior of particle-laden bubbles under asymmetric shear flow. Langmuir, 37, 13244.

S11-04: Interfacial flows

Date: June 2, 2023 08:30-10:30
Room: CHE/S91

Role of surface forces in wetting of rigid and soft substrates at the nanoscale

Kubochkin, Nikolai *(Technische Universität Darmstadt, Germany)* 08:30
Gambaryan-Roisman, Tatiana *(Technische Universität Darmstadt, Germany)*

Wetting science has advanced in understanding macro- and microscale processes in the last decades. However, wetting phenomena in systems of size comparable with the range of action of the intermolecular (surface) forces are not completely understood. In the present work, the wetting of rigid and soft substrates at the nanoscale is modeled for two configurations: propagation of a liquid rivulet within a wedge and evaporation of a nanoscale droplet. For both configurations, the wetting phenomena are modeled using a thin-film equation. The disjoining pressure concept is employed to take into account the influence of surface forces. The disjoining pressure isotherms include a nonretarded repulsive van der Waals term and an attractive electrostatic term. According to the classical theory of capillarity, if a liquid-gas interface is concave, a rivulet entering a wedge propagates indefinitely along its spine. We show that, when the surface forces are taken into account, the model predicts the formation of steady rivulets in the wedges in the case of a concave liquid-gas interface. Far from the entrance to the wedge, the steady-state solution approaches a limiting profile, which is determined by the gas humidity. The length of the rivulets between the entrance and the cross-section where the limiting profile is reached depends on the surface forces, humidity, and channel geometry. If the wedge walls are thin and deformable, the deflection of the walls depends on the wedge geometry and elastic modulus but is independent of the humidity. Droplet evaporation is considered for the case when the gas phase is comprised of pure vapor. We demonstrate that an evaporating droplet follows neither a constant contact angle nor a constant contact radius mode, but rather evaporates in a mixed mode. The deformability of a substrate leads to a reduction of the droplet's lifetime. The influence of the substrate deformability on the evolution of the contact angle is moderate.

Electrokinetic Modelling of Moving Contact Lines

Bauer, Lisa Sophie *(TU Darmstadt, Germany)* 09:10
Ratschow, Aaron D. *(TU Darmstadt, Germany)*
Hardt, Steffen *(TU Darmstadt, Germany)*

Charge accumulation of sliding droplets has been known for over two decades. Despite numerous experimental investigations, the physical mechanism of the charge separation is still poorly understood. Therefore, this investigation addresses the phenomenon with a numerical approach. When a solid is exposed to an electrolyte, a surface charge of bound ions is produced, and a diffuse layer of counter charges, the so-called Debye layer, arises. We identify the origin of charge separation at a receding contact line (CL) as the transfer of this immobilized surface charge from the wet to the dry region. Since the Debye layer structure is strongly affected by the gas-liquid interface as well as the fluid flow, the model focuses on ion

transport under creeping flow close to the receding CL, using the Stokes and Poisson-Nernst-Planck equations. Modelling the surface chemistry by means of a charge regulation model allows for a varying surface charge density that depends on the local ion concentration up to the CL. This is complemented by a transformation of the charge density profile at the solid surface to the frame-of-reference co-moving with the contact line. This implementation permits calculating the remaining immobilized surface charges at the receding CL and thus the degree of charge separation during dewetting. After performing a parameter study concerning surface chemistry, wetting and flow properties, we reveal the basic physical mechanism of charge separation for dewetting situations. Among others, we find that the charge transfer gets reduced with decreasing contact angle and increasing receding velocity.

How droplets pin on solid surfaces

Zhang, Jinming *(HZDR, Germany)*
Ding, Wei *(HZDR, Germany)*
Hampel, Uwe *(HZDR, Germany; TUD/IPE)*
09:30

When a droplet starts sliding on a solid surface, liquid-solid friction behaves in a manner comparable to solid-solid friction, that is, showing a static regime and a kinetic regime. Today, the kinetic friction force that acts on a sliding droplet is well-characterized. But the molecular mechanisms responsible for the static friction force are less understood. In this work, we use large-scale Molecular Dynamics (MD) simulations to investigate the static friction of a nano-droplet induced by nano-scale surface defects. We reveal three element-wise static friction forces related to the primary surface defects that can construct any complex surface defects and thus disclose the corresponding mechanisms of the static friction. In addition to the friction regime, we find that the resulting static friction law also shows an analogy to the solid-solid friction law. Our findings not only provide insight into the origin of the nano-scale contact line pinning phenomena but also lays a solid foundation for the understanding of wetting dynamics.

Droplets on elastic substrates - Numerical simulation of soft wetting

Aland, Sebastian *(TU Freiberg, Germany; HTW Dresden, Germany)*
09:50

Wetting of flexible substrates plays a major role in a broad variety of phenomena. The interaction between droplets and their surrounding is at small length scales dominated by surface tension forces. These forces may lead to significant deformation of the surrounding structure if either very soft or very thin. The interplay between wetting dynamics and structure mechanics leads to a range of fascinating phenomena from stick-slip motion to droplet-mediated remodeling of membranes. In this talk, we present a computational model which is capable to shed some light on such elastocapillary phenomena. The model captures the interaction between two immiscible fluids and a soft structure or membrane. The numerical method is based on a combination of a phase-field model with a moving finite-element grid. In numerical tests we demonstrate that this novel method is robust, flexible and accurate. We confirm analytical theory of droplet surfing on Kelvin-Voigt substrates and find an explanation

for the experimentally observed stick-slip phenomenon. Finally, we present first simulations of droplet-mediated membrane remodeling.

Modeling flow through tubes and annuli with liquid-infused surfaces for enhanced stability of the fluid-fluid interface

Zimmermann, Sebastian *(Micro Fluid Mechanics, RPTU Kaiserslautern-Landau, Germany)*
Bold, Ellen *(Physics and Technolgy of Nanostructures, RPTU Kaiserslautern-Landau, Germany)*
Oesterschulze, Egbert *(Physics and Technolgy of Nanostructures, RPTU Kaiserslautern-Landau, Germany)*
Chijiwa, Munehiro *(Photonik-Zentrum Kaiserslautern e.V., Kaiserslautern, Germany)*
Schäfer, Mareike *(Photonik-Zentrum Kaiserslautern e.V., Kaiserslautern, Germany)*
L'Huillier, Johannes *(Photonik-Zentrum Kaiserslautern e.V., Kaiserslautern, Germany)*
Schönecker, Clarissa *(Micro Fluid Mechanics, RPTU Kaiserslautern-Landau, Germany)*

10:10

Superhydrophobic and liquid-infused-surfaces (LIS) have been widely explored for their ability to reduce drag or to repel aqueous liquids. They rely on a second fluid (mostly air or oil) that is enclosed in the roughness features of a surface, which provides a slip boundary condition to the fluid flowing over the surface. The practical application of such surfaces is however challenged by this second fluid being pushed out of its place and thereby destroying the favorable properties of the surface.

We therefore investigate a new concept of superhydrophobic or LIS tubes that avoids these problems by employing „bottomless surfaces". These surfaces resemble a tube-in-tube configuration, where two different fluids flow through an inner tube and through an outer annulus.

In this contribution, we present the modelling of such surfaces. A description of the flow field can be obtained not only numerically, but also fully analytically based on a complex representation of the coupled inner and outer flows. The results present a basis for optimizing the geometry of the surface structures as well as the choice of the second fluid for a best performance.

S11-05: Interfacial flows

Date: June 2, 2023 11:00-13:00
Room: CHE/S91

The interplay of geometry and coarsening in multicomponent lipid vesicles under the influence of hydrodynamics

Bachini, Elena *(TU Dresden, Germany)*
Krause, Veit *(TU Dresden, Germany)*
Voigt, Axel *(TU Dresden, Germany)*

11:00

We consider the impact of surface hydrodynamics on the interplay between curvature and composition in coarsening processes on model systems for biomembranes. This includes scaling laws and equilibrium configurations, which are investigated by computational studies of a surface two-phase flow problem with additional phase-depending bending terms. These additional terms geometrically favor specific configurations. We find that as in 2D the effect of hydrodynamics strongly depends on the composition. In situations where the composition allows a realization of a
geometrically favored configuration, the hydrodynamics enhances the evolution into this configuration. We restrict our model and numerics to stationary surfaces and validate the numerical approach with various benchmark problems and
convergence studies.

A numerical approach for fluid deformable surfaces with conserved enclosed volume

Krause, Veit *(TU Dresden, Germany)*
Voigt, Axel *(TU Dresden, Germany)*

11:20

We consider surface finite elements and a semi-implicit time stepping scheme to simulate fluid deformable surfaces. Such surfaces are modeled by incompressible surface Navier-Stokes equations with bending forces. We here consider closed surfaces and enforce conservation of the enclosed volume. The numerical approach builds on higher order surface parameterizations, a Taylor-Hood element for the surface Navier-Stokes part, appropriate approximations of the geometric quantities of the surface and a Lagrange multiplier for the constraint. The considered computational examples highlight the solid-fluid duality of fluid deformable surfaces and demonstrate convergence properties, partly known to be optimal for different sub-problems.

A novel finite element formulation for thermal multi-phase flow including melting and evaporation with application to metal additive manufacturing melt pool modeling

Schreter-Fleischhacker, Magdalena *(Technical University of Munich, Germany)* 11:40
Much, Nils *(Technical University of Munich, Germany)*
Munch, Peter *(University of Augsburg, Germany)*
Kronbichler, Martin *(University of Augsburg, Germany)*
Wall, Wolfgang A. *(Technical University of Munich, Germany)*
Meier, Christoph *(Technical University of Munich, Germany)*

Metal additive manufacturing by laser powder bed fusion (LPBF) is a promising production technology, offering unique capabilities for on demand production of high performance metal parts with nearly unlimited freedom of design. However, the complex melt pool and vapor dynamics under typical process conditions can cause process instabilities, resulting in quality-degrading defects such as evaporation-induced pores, spatter, denudation, and lack of fusion. Hence, in-depth understanding of the physical phenomena of the laser-material interaction is crucial to obtain a complete picture of defect formation and eventually to fully exploit the potential of LPBF processes. Numerical models can help to enhance our understanding of the interplay between process parameters and part quality and can facilitate the advancement of processing methods [1].

While experimental investigations [2] have hypothesized that the majority of undesired pores are associated with evaporation-induced material redistribution dynamics, e.g., powder particle entrainment or also spattering, numerical melt pool models typically consider evaporation only through simplified models by taking into account the evaporation-induced pressure jump and neglecting the evaporation-induced flow [3]. Our contribution focuses on accurately modeling the interplay between dynamics of the melt pool and the vapor jet of LPBF based on a mesoscale multi-phase model, including melt pool formation and the interaction of the multi-phase system solid metal, liquid metal and metal vapor. In our talk, we present an advanced modeling approach by considering the evaporation-induced volume expansion and the resulting mass flux across the liquid-vapor interface in addition to the evaporation-induced pressure jump. In the medium term, this will provide new insights into crucial physical effects on the mesoscale, some of which are challenging to measure experimentally.

Our multi-phase model is formulated using an Eulerian framework. We employ a conservative level set formulation to track the diffuse metal-vapor interface, allowing us to naturally capture a priori unknown moving interfaces and complex topology changes of the metal-vapor interface, such as keyholes, gas pockets, spattering, etc. For time discretization, we use semi-implicit time stepping schemes. Space discretization is performed using finite elements with an adaptively refined mesh, guaranteeing a high spatial resolution of the interface region. In combination with highly efficient matrix-free solvers based on sum-factorization techniques, our modeling framework is capable of simulating practically relevant time and length scales.

[1] Meier, C., et al., GAMM-Mitteilungen 44.3 (2021): e202100014.
[2] Bitharas, I., et al., Nature Communications 13.1 (2022): 2959.
[3] Khairallah, S. A., et al., Acta Materialia 108 (2016): 36-45.

Simulations for Two-Phase Flows in Injection Molding Processes

Ferrer Fabón, Blanca *(RWTH Aachen University, Germany)*
Behr, Marek *(RWTH Aachen University, Germany)*
12:00

High-resolution numerical simulations of polymer injection molding are crucial for preventing manufacturing defects during this process. However, the challenges in such simulations are manifold, and efficient high-resolution numerical analysis is still subject to research.

In this study, we build a macro-scale numerical description of the melted polymer during the filling phase. We use the in-house finite-element solver XNS to simulate the polymer and air flows as an interfacial flow, utilizing the level-set method. A two-phase flow always involves high discontinuities across the interface; consequently, a high mesh resolution along the interface is needed. Another difficulty in the injection molding simulation is the non-linearity introduced by the melted polymer properties, such as the shear-thinning and pvT models. Additionally, our model is extended to semi-crystalline polymers with a novel adaptation of the non-isothermal crystallization kinetics. These and more complexities of the model are presented, and the simulation results and performance are analyzed.

Influence of different pipe wall and flushing liquid temperature on flushing behavior of highly viscous fluids

Liebmann, Vera *(TU Dresden, Chair of Fluid Mechanics Germany, 01062 Dresden)*
Heide, Matti *(TU Dresden, Chair of Processing Machines and Processing Technology, 01062 Dresden)*
Köhler, Hannes *(TU Dresden, Chair of Processing Machines and Processing Technology, 01062 Dresden)*
Rüdiger, Frank *(TU Dresden, Chair of Fluid Mechanics Germany, 01062 Dresden)*
Fröhlich, Jochen *(TU Dresden, Chair of Fluid Mechanics Germany, 01062 Dresden)*
12:20

In recent years, the food industry has seen a large increase in product variety. Instead of dedicated lines producing a single product, most lines now have to produce a large variety of products in rapid succession. Cleaning is required between each product change. For highly viscous fluids a widely applied cleaning process, particularly for pipework, is flushing. It entails the displacement of previous product using follow-up product. If both products are non-mixing, the flushing process may be described purely by the movement of the interface of the two products. This is mainly influenced by the rheology of both products, the process parameters, e.g. massflow and temperature, and the dimensions of the parts to be cleaned.

In this contribution the authors investigate how flushing of chocolate using a follow-up chocolate in a simple pipe is affected by temperature. The authors investigate a non-uniform distribution of temperature across the considered domain. This is done using two cases, where the first will exhibit a wall temperature deviating from the normal process temperature and the second will exhibit a differently tempered follow-up chocolate. The investigations are performed using unsteady three-dimensional numerical simulations with one of OpenFOAM's multiphase solvers, which is extended to include an additional equation for energy conservation. The physical properties of the chocolate are analyzed with respect to their dependence on temperature and implemented in a new model in OpenFOAM.

The results of both cases are assessed according to industrially relevant questions. Among others, these include the amount of follow-up chocolate needed to achieve a set goal of cleanliness. The time needed to achieve this is also considered. A dimensionless time is used to compare the different cases. Finally, the authors give recommendations on how using different temperature of pipe wall and follow-up chocolate may lead to improved flushing processes and which savings may be achieved with this strategy.

A magnetically-activited fluidic based thermal switch

Michak, Robin *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf (HZDR),Bautzner Landstrasse 400, 01328 Dresden, Germany)*
Ortmann, Kilian *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf (HZDR),Bautzner Landstrasse 400, 01328 Dresden, Germany)*
Lei, Zhe *(Institute of Fluid Dynamics, Helmholtz-Zentrum Dresden-Rossendorf (HZDR),Bautzner Landstrasse 400, 01328 Dresden, Germany; Institute of Process Engineering and Environmental Technology,Technische Universität Dresden, 01062 Dresden, Germany)*

12:40

Alternative cooling technologies such as solid state refrigeration is well known due to its merit in its zero nominate global warming potential and ozone depletion potential. When the thermal energy is generated at a solid state refrigerant from an externally applied magnetic source, e.g. in magnetic cooling and multicaloric cooling, the operation is theoretically more efficient, silent as well as compact. Besides, the thermomagnetic generator gains increasing attention as it meets the technological demand in low grade waste heat energy ($\leq$ 232 degree C) harvesting. Both the magnetic cooling and thermomagnetic generator are enabled with a type of material called magnetocaloric material (MCM). It possesses the feature of having a thermal effect when exposed to a temporally varying magnetic field. The common MCM has a maximum room temperature magnetocaloric effect of O(1 K/ T). This intrinsic parameter, determined by material property, limits the direct application in temperature span which is more than one order of magnitude higher for both the refrigeration cycle (e.g. fridge or residential building cooling ~ 10-30 K) and the low grade energy source. To expand the temperature span, MCM is used simultaneously as a regenerator and realized commonly by an active magnetic regenerator principle. Thus, the cooling load is generated at each oscillation cycle of magnetization and fluid flow. However, the reciprocating flow contributes as a major energy loss and prevent the cycling from operating in higher frequency. To improve the current AMR based system's efficiency, one idea is to embed a thermal switch that selectively allows directional heat transfer depending on the magnetization/demagnetization phase of the MCM. Hence, a uni-directional heat transfer fluid flow, delivers less pumping loss, can replace the reciprocating one and give rise to an elevated working efficiency. We present here a design of a fluidic based thermal switch constituted of a thermally insulating air and a thermally conductive water connecting two thermal ends. A good thermal insulation is ensured by the thin air film that naturally phase separated with that of water. At an elevated magnetic stray field, comes naturally from magnetic cooling and thermomagnetic generator, the flux density addresses the paramagnetic property that is seeded into the water phase and

cause interface flow that thermally “short-cut” the two ends, hence an elevated heat flux. The transient and steady state thermal evaluation is covered that serves as a key parameter for numerical simulations for system level design and optimization.

S11-06: Interfacial flows

Date: June 2, 2023 16:00-18:00
Room: CHE/S91

Diffuse-interface incompressible fluid mixture models

ten Eikelder, Marco *(TU Darmstadt, Germany)* 16:00
van der Zee, Kristoffer *(University of Nottingham, UK)*
Schillinger, Dominik *(TU Darmstadt, Germany)*

Many diffuse-interface Navier-Stokes Cahn-Hilliard (NSCH) models with non-matching densities have been proposed over the last decades, see e.g. [1,3]. Even though these models aim to represent the same physical phenomena, they are (seemingly) different. The first objective of this talk is to present a framework for NSCH models that unites all of these models [2]. This framework relies on mixture theory of rational mechanics and completes the fundamental exploration of alternate non-matching density NSCH models.

The NSCH model with non-matching densities is not fully incompatible with mixture theory. Namely, it is a reduced model that in which the evolution equations for the diffusive fluxes are replaced by constitutive models. The second objective of this talk is to present an incompressible model that fully compatible with mixture theory. This model may be formulated either in constituent or in mixture quantities. With this observation it may be directly compared to the NSCH model, which reveals the inconsistencies of the incompressible NSCH model with rational mixture theory.

[1] Abels, H., Garcke H. and Grün, G., Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities, Mathematical Models and Methods in Applied Sciences, (2012) 22: 1150013.

[2] ten Eikelder, M.F.P., van der Zee, K.G., Akkerman, I. and Schillinger, D., A unified framework for Navier-Stokes Cahn-Hilliard models with non-matching densities. Mathematical Models and Methods in Applied Sciences (2022), https://doi.org/10.1142/S0218202523500069.

[3] Lowengrub, J.S., Truskinovsky, L., Quasi-incompressible Cahn-Hilliard fluids and topological transitions, Proceedings of the Royal Society of London. Series A: Mathematical, Physical and Engineering Sciences, (1998) 454: 2617–2654.

A Numerically Consistent Unstructured Volume-of-Fluid Discretization for the Two-Phase Momentum Convection with High-Density Ratios

Liu, Jun *(Technischen Universität Darmstadt, Germany)* 16:20
Tolle, Tobias *(Robert Bosch GmbH, Germany)*
Scheufler, Henning *(DLR German Aerospace Center, Institute of Space Systems, Germany)*
Zuzio, Davide *(The French Aerospace Lab ONERA, France)*
Estivalezes, Jean-Luc *(The French Aerospace Lab ONERA, France)*
Bothe, Dieter *(Technischen Universität Darmstadt, Germany)*
Marić, Tomislav *(Technischen Universität Darmstadt, Germany)*

We extend the numerically consistent discretization of the single-field two-phase momentum convection from the ρLENT method - an unstructured Level Set / Front Tracking method

- to the isoAdvection VOF method. The numerical consistency of the momentum convection term in the discretized single-field Navier-Stokes equations is crucial for the numerical stability when simulating two-phase flows with high density ratios. We use an auxiliary mass transport equation to ensure the numerical consistency. A careful derivation of the unstructured VOF discretization indicates that an exact solution of the volume fraction equation is equivalent to solving this auxiliary mass equation. However, equation discretization is unavoidable, and it introduces the inequality between the numerical integration of the mass flux $\rho_f F_f$ and the geometrical integration of the phase-specific volume by the VOF method. Two numerically consistent discretizations are possible with the isoAdvection VOF method. First, an auxiliary mass equation can be solved, while carefully dealing with the face-centered density. Second, an appropriate discretization scheme chosen for the momentum convection term stabilizes the solution. Multiple droplet studies with the density-ratio range $\rho^- / \rho^+ = [1, 10^6]$ are used to verify the discretization.

Curvature approximation for the unstructured geometrical VOF method

Chai, Guoliang *(Mathematical Modeling and Analysis, TU Darmstadt, Germany)* 16:40
Liu, Jun *(Mathematical Modeling and Analysis, TU Darmstadt, Germany)*
Tolle, Tobias *(Corporate Research, Robert Bosch GmbH, Germany)*
Lippert, Anja *(Corporate Research, Robert Bosch GmbH, Germany)*
Bothe, Dieter *(Mathematical Modeling and Analysis, TU Darmstadt, Germany)*
Marić, Tomislav *(Mathematical Modeling and Analysis, TU Darmstadt, Germany)*

We propose a novel interface curvature approximation algorithm for the unstructured geometrical VOF method that relies on the Iterative Defect Correction method. The algorithm uses the PLIC normals to construct a Reconstructed Distance Function (RDF) in interface-cells and the first point-cell neighborhood. This results in a smooth RDF field whose discrete finite volume gradient delivers interface-normals in interface-cells. Interface-normals computed this way provide a sufficiently regular vector field for the unstructured finite volume divergence operator to compute the mean curvature in the interface-cell layer.

The finite volume discretization of the Continuum Surface Force surface tension model requires a constant mean curvature in the interface-normal direction. The curvature at PLIC polygon centroids is interpolated from the mean curvature associated to interface-cell centers and extrapolated back to the corresponding interfacial-cell centres. Therefore, the extrapolation method developed for the interface-normal vector field extrapolates mean curvature from PLIC polygon centroids into one layer of face-neighbour cell centres. This algorithm is implemented as a curvature model in the TwoPhaseFlow project, a state-of-the-art implementation of the geometrical VOF in the OpenFOAM open-source software. Results show that our proposed algorithm outperforms other curvature models, given a sufficiently resolved curvature.

S12: Waves and Acoustics

Organizer(s): **Langer, Sabine** *(TU Braunschweig)*
Schanz, Martin *(TU Graz)*

S12-01: Waves and Acoustics

Date: June 1, 2023 08:30-10:30
Room: CHE/184

Elastic tracking of dynamic viscoelastic displacements by actuation stress: Theory and 1D analytic example involving shock waves

Irschik, Hans *(Johannes Kepler University of Linz, Austria)* 08:30
Krommer, Michael *(Johannes Kepler University of Linz, Austria)*

Our study is concerned with the tracking, or morphing, of force-induced dynamic displacements in linear elastic solids and structures by means of actuating eigenstrains, i.e. we seek for a transient spatial distribution of additional eigenstrains, such that the total displacement of the elastic structure coincides with the displacement field to be tracked. The action of eigenstrains is characterized by actuation stresses. The present authors and their co-workers have contributed to this tracking problem in a series of papers, see e.g. [1] and the literature cited there. The related problem of developing numerical schemes for finding additional eigenstrains that act upon a linear elastic structure, such that corresponding dynamic inelastic displacements are generated, has been treated by the senior author and his co-authors before, see [2] for an overview on thermo-viscoplastic problems. Such a numerical scheme allows to utilize convenient linear computational solution procedures in a non-linear setting. In the present study, as a contribution to the linear theories of elasticity and viscoelasticity, we focus on analytic formulations. First, we extend the tracking theory with respect to the presence of propagating singular wave fronts. As a closed form analytic example, we then study the uni-axial (1D) deformation of a linear elastic half-space under the action of a suddenly applied surface traction, which induces a uni-axial shock wave that propagates into the half-space. The present tracking goal is to add to the surface traction a transient spatial distribution of actuation stress such that the total elastic displacement coincides with the shock wave produced by the surface traction in a viscoelastic half-space. In order to obtain closed form solutions, symbolic computation is used and a Maxwell material is considered. The converse problem, namely to apply an actuation stress to a viscoelastic structure such that the corresponding dynamic displacements in a linear elastic structure are obtained has been recently studied in [3].

[1] H. Irschik, M. Krommer and Ch. Zehetner, “Displacment tracking of pre-deformed smart structures”, *Smart Structures and Systems*, vol. 18, pp. 139-154, 2016.
[2] H. Irschik and F. Ziegler, “Dynamic processes in structural thermo-viscoplasticity,” *Applied Mechanics Reviews*, vol. 48, pp. 301-316, 1995.
[3] H. Irschik, M. Krommer, “Dynamic Displacement Tracking in Viscoelastic Solids by Actuation Stresses: One-Dimensional Analytic Example Involving Shock Waves”, *Bulletin of the Polish Academy of Sciences, Technical Sciences (BPASTS)*, to appear, 2023.

Modeling Elastic Waves in Unbounded Domains using Peridynamics

Shojaei, Arman *(Helmholtz-Zentrum Hereon, Germany)* 09:10
Hermann, Alexander *(Helmholtz-Zentrum Hereon, Germany)*
Cyron, Christian J. *(Hamburg University of Technology)*

This presentation will provide an in-depth look into the use of peridynamics (PD) for the study of the propagation of elastic waves in unbounded domains. The main focus of the presentation will be on the development of absorbing boundary conditions (ABCs) that are derived from a semi-analytical solution of the PD governing equation in the exterior region. This solution consists of a finite series of plane waves, known as fundamental solutions or modes, that satisfy the PD dispersion relations. The unknown coefficients of the series are then determined through a collocation procedure at subregions around each absorbing point.

One of the main advantages of the proposed ABCs is that they are of Dirichlet-type, making them simple to implement as they do not require derivatives of the field variables. Additionally, the ABCs are constructed in both the time and space domains, eliminating the need for cumbersome Fourier or Laplace transforms that are often required for nonlocal models. The modes used in the solution also satisfy the same numerical dispersion relations as the near field, ensuring compatibility between the far-field and near-field solutions.

The performance of the proposed ABCs will be evaluated through several examples, including problems characterized by highly-dispersive propagating waves such as crack propagation in brittle solids. The results of these simulations will demonstrate the stability of the proposed ABCs in time and their ability to maintain an appropriate level of accuracy even in complex problems.

Overall, this presentation will provide valuable insights into the application of peridynamics for the study of elastic wave propagation in unbounded domains. The proposed absorbing boundary conditions will be shown to offer significant advantages over other existing methods, making them a promising tool for future studies in this field.

Hydrodynamic Forces Acting on Mechanical Systems in Linear and Nonlinear Ocean Waves

Hollm, Marten *(Hamburg University of Technology, Germany)* 09:30
Seifried, Robert *(Hamburg University of Technology, Germany)*

In the real ocean, there are various ships and offshore structures that differ in their geometric shape and in the depth of water into which they reach. When they are constructed, the safety limits must be determined. For this, the hydrodynamic forces acting on the various mechanical structures have to be known. In order to compute the acting forces occurring in oceans as accurate as possible, the corresponding sea states and fluid structure interactions have to be modeled in the same way. This can be done solving the Euler equations of fluid mechanics. However, since they are highly nonlinear, it is computationally very expensive to solve them. In order to simplify the problem, Taylor series expansions are used to approximate them by linear and nonlinear wave theories. This results in Stokes wave theories of different orders. While it is computationally cheap to deal with the linear wave theory, the corresponding results are only accurate for small wave amplitudes. For higher wave amplitudes, nonlinear wave theories have to be used. However, in an irregular sea state consisting of several harmonic wave components, interactions between the different components have

to be considered. This makes the solving of the nonlinear theories computationally more expensive.

In the present work, the hydrodynamic forces acting on prescribed free-floating mechanical systems are studied. Regular as well as irregular sea states are considered using Stokes wave theory of first, second and third order. It is analyzed how much the magnitude and temporal behavior of the forces can differ using nonlinear theories of different orders instead of the linear wave theory. The corresponding effects on the dynamics of the mechanical system are investigated. Thereby, the fluid structure interaction and hydrodynamic forces are computed solving the corresponding partial differential equations of the linear and nonlinear wave theory. In this way, the nonlinear interactions of the different wave components in irregular seas and the disturbances of the sea due to the presence of the mechanical system are captured.

An approach for improving SHM systems with guided ultrasonic wave detection and embedded sensors by a planar gradient acoustic impedance matching

Rottmann, Max *(Helmut-Schmidt-University, Hamburg, Germany)* 09:50
Weber, Wolfgang E. *(Helmut-Schmidt-University, Hamburg, Germany)*

For technical structures, such as airplanes, the service life must be increased to satisfy the requirements for high efficiency in terms of costs and sustainability. Monitoring the system's current health and providing solutions to maintain it reliably is one way to accomplish this objective. A structural health monitoring system, in which actuators induce a guided ultrasonic wave or wave-field monitored by a sensor or a network of sensors, is a standard for thin-walled structures, which are made of e.g. fibre-metal-laminates. The sensor measurements provide information that can be used to determine the respective health state of the system. However, embedding the actuator and sensors in the system typically results in a distortion of the wave-field e.g. mode-conversion and reflections. The distortion can lead to over- or underestimation of the quantity, location, and severity of the damage. Due to these false-detections, both an unnecessary high effort for retrofitting the structure and a reduction of the structure's technical reliability may be needed. The objective of the current contribution is to reduce the wave-field distortion/reflections caused by the sensors to prevent or minimise these false-detections. To reduce the distortion and reflection of the wave-field, a functionally graded material with an acoustic impedance matching based on a mechanical model is used. In order to control and adjust the acoustic impedance, which is the leading parameter concerning distortion and reflections of waves, tungsten particles were added to the uncured epoxy resin. The design of an interphase between the sensor or its glass housing and the surrounding structure is achieved by this novel approach. The interphase properties are varying in the radial direction to the sensor and are depending on the tungsten particle content in the epoxy resin. In this work, several models regarding the radial distribution of the tungsten particle content and the excitation frequency are investigated. Additionally, the dependence on various mode shapes, such as symmetric and antisymmetric modes, is also addressed. The approach results, for specific configurations, in (I) reduced reflections from the sensor (less

distortion) and (ii) amplified measuring signals of the sensor. Numerous numerical examples demonstrate the benefit of the presented approach.

S12-02: Waves and Acoustics

Date: June 2, 2023 08:30-10:30
Room: CHE/184

Multi-fidelity Gaussian Processes for an efficient approximation of frequency sweeps in acoustic problems

Gürbüz, Caglar *(Technische Universität München, Germany)* 08:30
Marburg, Steffen *(Technische Universität München, Germany)*

Highly accurate predictions from large-scale numerical simulations are mostly associated with increased computational resources and time expense. As a consequence, the data generation process can only be performed for a small sample size limiting a detailed investigation of the underlying system. The concept of multi-fidelity modeling allows to combine data from different models of varying costs and complexity. This study introduces a multi-fidelity model for the acoustic design of a vehicle cabin. Therefore, two models with different fidelity levels are used to solve the Helmholtz equation at specified frequencies with the boundary element method. Gaussian processes are trained on each fidelity level with the simulation results to predict the unknown system response. By this means, the multi-fidelity model enables an efficient approximation of the frequency sweep in acoustic analyses within the frequency domain. Additionally, the proposed method inherently quantifies uncertainties due to the random nature of the data generation process. To demonstrate the effectiveness of our framework, the approximation of the frequency sweep is validated with the high-fidelity solution at each frequency. The results show that the frequency sweep is efficiently approximated by using only a very small number of high-fidelity simulations. Thus, our findings indicate that multi-fidelity Gaussian processes can be adopted for fast and, at the same time, accurate predictions.

Realizations of the Generalized Adaptive Cross Approximation in an Acoustic Time Domain Boundary Element Method

Schanz, Martin *(Graz University of Technology, Austria)* 08:50

In acoustics the boundary element method (BEM) is much more common compared to elasticity. This is driven by the applications, which are in acoustics very often radiation problems causing trouble in finite element or finite volume methods. Nevertheless, for a time domain calculation still an efficient BE formulations is lacking. We consider the time domain BEM for the homogeneous wave equation with vanishing initial conditions and given Dirichlet and/or Neumann boundary conditions. The generalized convolution quadrature method (gCQ) developed by Lopez-Fernandez and Sauter [2] is used for the temporal discretisation. The spatial discretisation is done classically. Essentially, the gCQ requires to establish boundary element matrices of the corresponding elliptic problem in Laplace domain at several complex frequencies. Consequently, an array of system matrices is obtained. This array of system matrices can be interpreted as a three-dimensional array of data which should be approximated by a data-sparse representation. The Adaptive Cross Approximation (ACA) can be generalized to handle these three-dimensional data arrays [1]. The basic idea is the same as for the original algorithm. Adaptively, the rank of the three-dimensional data array is increased until a

prescribed accuracy is obtained. On a pure algebraic level it is decided whether a low-rank approximation of the three-dimensional data array is close enough to the original matrix. Hierarchical matrices are used in the two spatial dimensions and the third dimension are the complex frequencies. Hence, the algorithm makes not only a data sparse approximation in the two spatial dimensions but detects adaptively how much frequencies are necessary for which matrix block. In the presentation this methodology is recalled and applied either to the H-matrix as a whole or for each block within the H-matrix. Some examples will show how the method performs.

[1] M. Bebendorf, A. Kuhnemund, and S. Rjasanow, An Equi-Directional Generalization of Adaptive Cross Approximation for Higher-Order Tensors. Applied Numerical Mathematics 74 (2013), pp. 1-16
[2] M. Lopez-Fernandez and S. Sauter, Generalized Convolution Quadrature with Variable Time Stepping. IMA Journal of Numerical Analysis 33 (2013), pp. 1156-1175

Partial Integration based Regularization in Fast Multipole Boundary Element Method

Lakshmi Keshava, Vibudha *(Institute of Applied Mechanics, Graz University of Technology, Technikerstraße 4, Graz 8010, Austria)*
Schanz, Martin *(Institute of Applied Mechanics, Graz University of Technology, Technikerstraße 4, Graz 8010, Austria)*

09:10

The boundary element method (BEM) has proven to be a highly effective numerical method for solving elasticity problems in both 2D and 3D. It has several benefits, including its accuracy in modeling stress concentrations, as well as its simplicity in dealing with complicated elastic domains. However, BEM also has several challenges that need to be addressed, such as the presence of singular kernels or the computationally expensive dense system matrices. Several regularization techniques have already been developed and applied to overcome the former. One such method uses partial integration (Stokes theorem) to transform hyper-singularities and the strong singular integral kernels into weakly singular integral kernels. The latter issue of BEM being computationally expensive can be dealt with certain fast methods. One way to reduce memory and computational cost is by using the Chebyshev interpolation-based fast multipole method (FMM). When the above mentioned Stokes theorem-based regularization technique is combined with the Chebyshev interpolation-based FMM, a problem arises at the boundary of the near-field and far-field interactions. This problem results from the boundary terms generated by partial integration and the different treatments of the near-field and far-field kernels. We present a new solution to this problem by implementing partial integration on all kernels and then utilizing the Chebyshev interpolation-based FMM on the transformed kernels. By doing so, the boundary terms from partial integration are effectively mitigated and the different treatments of the near-field and far-field kernels are made uniform. We have considered a 3D elastostatic problem with direct BEM formulation using the collocation method to verify this method and approve its robustness and reliability.

Adaptive time stepping for generalized Convolution Quadrature

Balagopal Menon, Arjun *(Institute of Applied Mechanics, Graz University of Technology, Technikerstraße 4, A-8010 Graz, Austria)* 09:30
Schanz, Martin *(Institute of Applied Mechanics, Graz University of Technology, Technikerstraße 4, A-8010 Graz, Austria)*

Through the current work we aim to improve the Boundary Element method in acoustics. The proposed adaptivity is based on the time domain Boundary Element formulation. In this setting, an elegant method for solving the acoustic problem is through the transformation of the underlying partial differential equation on to the boundary of the domain as a space time boundary integral equation. Furthermore, for such space-time problems, it is desirable to investigate a non-uniform step size in the time domain to account for the irregularities and localized variations in the temporal solution. This ensures that the number of times steps is reasonable while also speeding up the numerical solution.

The boundary element integral equation in the time domain has a convolution in time which is numerically solved using a convolution quadrature method. For the implementation of an adaptive step size the generalized Convolution Quadrature method (gCQ)[1] is then used. The gCQ method under consideration uses a higher order time stepping method, like the Runge Kutta method. This will achieve a higher order in time for the space-time boundary element method as long as there is a sufficiently good spatial discretization.It has been established that variable step size can be introduced for numerically solving Ordinary Differential Equations (ODEs) with the help of error estimators. The gCQ reduces the convolution problem into a coupled system where an ODE governs the time behavior. The adaptivity in time domain is achieved by defining an error and keeping the local error within a prescribed tolerance. The current work shows that an approach similar to that of the ODEs can be included in the gCQ to introduce an adaptive control of the time step size in the 3D boundary element formulation.

[1] López-Fernández M., Sauter S., *Generalized convolution quadrature with variable time stepping*. IMA Journal of Numerical Analysis, 33 (4): 1156-1175, 2013.

Efficient solutions of preconditioned large-scale systems for simulative aircraft noise assessment

Hüpel, Yannik *(Institute for Acoustics, TU Braunschweig, Germany)* 09:50
Blech, Christopher *(Institute for Acoustics, TU Braunschweig, Germany)*
Sreekumar, Harikrishnan K. *(Institute for Acoustics, TU Braunschweig, Germany)*
Langer, Sabine C. *(Institute for Acoustics, TU Braunschweig, Germany)*

The rising number of passengers transported by aircraft leads to more flight traffic, further increasing the environmental impact of the aviation sector. In order to combat the growing environmental impact, the Cluster of Excellence Sustainable and Energy Efficient Aviation of TU Braunschweig aims to advance research towards a climate neutral aviation industry, especially with the design of newly developed aircraft. In the conscience of passengers, the focus is also shifted towards a healthy and comfortable travel experience. One of the main factors influencing these aspects is noise inside the aircraft cabin. A lower noise impact can help increase the technology acceptance and further push towards more sustainable airborne transport solutions.

In order to assess cabin noise with moderate effort in an early design stage, simulative methods such as the Finite Element Method (FEM) are deployed. These have the advantage of yielding important insights into the noise distribution inside the aircraft cabin without having to have a built prototype present. Since methods like the FEM are of a wave-resolving nature, results contain high resolution wave propagation information of the soundwaves, created, for example by the excitation of the turbulent boundary layer on the aircraft's outer skin. Additionally, a direct auralisation at seat positions is possible. More powerful computers have further improved the usage of models for an early design noise assessment. However, the more elaborate a model is, the more Degrees of Freedom (DOFs) it yields as final system of equations. Finally, since the FEM is of wave-resolving nature and in order depict sound waves accurately, a fine discretization of 10 nodes per frequency dependent wave length is needed. This leads to a massive increase in DOFs for higher frequencies and finally yielding a large-scale model, which entails huge computational efforts. This makes the usage of adaptive grids very convenient. In this contribution, adaptive grids entail two main aspects: Frequency and domain adaptive discretization. Since higher frequencies lead to shorter wavelengths and therefore finer mesh sizes it is feasible to adaptively discretize the model in the frequency domain, while also adaptively discretizing the different domains of the models itself, because different materials lead to different wavelengths. However, the resulting system of equations might be ill-posed. Therefore, this contribution aims to shed light on an efficient solving process of these adaptively discretized large-scale models with preconditioning and adequate solver choice.

S12-03: Waves and Acoustics

Date: June 2, 2023 11:00-13:00
Room: CHE/184

Multi-metamaterial structures via the reduced relaxed micromorphic model

Perez Ramirez, Leonardo Andres *(TU Dortmund, Germany)* 11:00
Rizzi, Gianluca *(TU Dortmund, Germany)*
Voss, Jendrik *(TU Dortmund, Germany)*
Madeo, Angela *(TU Dortmund, Germany)*

Metamaterials allow us to go beyond the limitations of traditional materials. In fact, their ability to exhibit properties that do not usually occur in classical materials has gained them increasing attention in the last decades. For example, in the field of mechanical metamaterials, tailoring the geometry of the underlying microstructure can result in negative constitutive parameters and exotic interactions with elastic waves (focusing, channeling, cloaking, band gaps, and more). However, simulating the response of these systems proves challenging. In the case of metamaterials that have band gaps, i.e., frequency ranges for which wave propagation is inhibited, the traditional Cauchy continuum theory fails to capture the dispersive response of the material, and higher-order models and enriched kinematics models appear as alternatives. The relaxed micromorphic model [3] belongs to the latter category and has been shown to capture the macroscopic behavior of a large class of metamaterials, including band gaps [1]. We show in this work how it can be used to simulate not only the response of metamaterials, but also the interactions of classical materials with metamaterials at finite sizes. Two instances are presented here, a double-shield structure designed to widen the effective range of the band gap, and a multiple-shield structure that explores the screening in regions internal and external to single-shields [2]. Both instances of multi-element metamaterials are embedded in a classical Cauchy continuum. The dynamical response of both systems is studied with the finite element implementation of the reduced relaxed micromorphic model. Additionally, the results are checked against direct simulations of the full-microstructure. We find that the reduced relaxed micromorphic model captures well the response of the metamaterial structures, including the interaction with the classical Cauchy material, at a fraction of the computational cost of the direct simulations of the full-microstructure.

[1] D'Agostino, M., Barbagallo, G., Ghiba, I., Eidel, B., Neff, P. & Madeo, A. Effective Description of Anisotropic Wave Dispersion in Mechanical Band-Gap Metamaterials via the Relaxed Micromorphic Model. Journal Of Elasticity. 139, 299-329 (2020)
[2] Perez Ramirez, L., Rizzi, G. & Madeo, A. Multi-element metamaterial's design through the relaxed micromorphic model. ArXiv Preprint. https://arxiv.org/abs/2210.14697. (2022)
[3] Neff, P., Ghiba, I., Madeo, A., Placidi, L. & Rosi, G. A unifying perspective: The relaxed linear micromorphic continuum. Continuum Mechanics And Thermodynamics. 26, 639-681 (2014)

Modeling wave propagation in a finite-size metamaterial through a reduced relaxed micromorphic model.

Demetriou, Plastiras *(TU Dortmund, Germany)* 11:20
Voss, Jendrik *(TU Dortmund, Germany)*
Rizzi, Gianluca *(TU Dortmund, Germany)*
Madeo, Angela *(TU Dortmund, Germany)*

In the last decades, the research towards the identification and characterization of metamaterials with exotic properties has seen a significant expansion. The main challenge to face in order to model such materials is the heavy computational cost that is required to simulate large domains, especially since these materials are often characterised by an intricate geometry. To circumvent this limitation, it is here proposed the use of an equivalent enriched model (a reduced relaxed micromorphic model [1, 2]) which is based on a variational formulation that automatically guarantees the well posedness of the model and provides appropriate boundary conditions. The latter are essential to properly model finite size samples. Simulations are carried out to test the capability of such model to mimic the response of a finite-size microstructured material for a wide range of frequencies. The different metamaterials characterised in this work are obtained with the periodic repetition of different unit cells with tetragonal symmetry and made up of either polymers (e.g. plexiglass) or metals (e.g. titanium). All of these metamaterials have a band-gap in the acoustic range, which makes them particularly suitable for soundproofing applications.

[1] Demore, F., Rizzi, G., Collet, M., Neff, P. & Madeo, A. Unfolding engineering metamaterials design: Relaxed micromorphic modeling of large-scale acoustic meta-structures. Journal Of The Mechanics And Physics Of Solids. 168 pp. 104995 (2022)
[2] Rizzi, G., Neff, P. & Madeo, A. Metamaterial shields for inner protection and outer tuning through a relaxed micromorphic approach. Philosophical Transactions Of The Royal Society A. 380, 20210400 (2022)

Improved sound absorption characteristics of a novel porous metamaterial structure

Liu, Qihang *(University of Siegen, Germany)* 11:40
Zhang, Chuanzeng *(University of Siegen, Germany)*

The sound absorption characteristics of a novel porous metamaterial structure for obliquely incident acoustic waves are studied in this work. The novel porous metamaterial structure is composed of a periodic porous matrix and periodically distributed adjacent second-type porous layers containing slits. The theoretical model is established by applying the double porosity theory to the second-type porous layer and the slit which forms an equivalent inclusion, and then the homogenization method is applied to the porous metamaterial structure which can be described by a unit-cell composed of a porous matrix containing the equivalent inclusion. The theoretical results are validated by the numerical results obtained by the finite element software COMSOL Multiphysics and fairly good agreements are achieved. Several examples demonstrate the improved sound absorption characteristics of the porous metamaterial structure for various angles of the obliquely incident acoustic waves. Furthermore, the

acoustic impedance and the time-averaged power dissipation density are also investigated and will be reported to gain a better understanding of the sound absorption mechanisms.

Towards the use of a reduced order and stochastic turbulence model for assessment of far-field sound radiation: low Mach number jet flows

Medina Méndez, Juan A. *(BTU Cottbus-Senftenberg, Chair of Numerical Fluid and Gas Dynamics)*
Sharma, Sparsh *(BTU Cottbus-Senftenberg, Chair of Numerical Fluid and Gas Dynamics; University of Cambridge, Department of Applied Mathematics and Theoretical Physics)*
Schmidt, Heiko *(BTU Cottbus-Senftenberg, Chair of Numerical Fluid and Gas Dynamics)*
Klein, Marten *(BTU Cottbus-Senftenberg, Chair of Numerical Fluid and Gas Dynamics)*

12:00

Turbulence is an important source of sound radiation. Lighthill formulated the equations for sound generation back in the 1950s [1]. However, it is only recently that the available computational power has allowed detailed numerical evaluations reaching moderate Reynolds numbers, like the Direct Numerical Simulation (DNS) of a subsonic jet by Wang et al. [2]. Unfortunately, the high cost of DNSs makes it unfeasible to simulate large Reynolds number flows. This is a task that could be achieved by reduced order models, e.g., the map-based stochastic One-Dimensional Turbulence (ODT) model. The ODT model has been applied to several flow configurations, among others, to low Mach number turbulent jet flows [3]. We aim to predict spectra of pressure fluctuations in the acoustic far field generated by a localized low Mach number turbulent jet. To that extent, we model the time-dependent velocity fluctuations in the acoustic near field by fully resolving all relevant scales of the flow along the radial coordinate (jet diameter) using the ODT model. We consider the wave equation for the acoustic pressure p following [4], derived by a combination of the temporal derivative of the continuity equation and the divergence of the inviscid momentum equation for isentropic flow of an ideal gas,

$(1/c_0^2)\,\partial^2 p/\partial t^2 - \Delta p = S.$

On the left hand side, c_0 is the speed of sound in the (far-field) reference thermodynamic state (fluid at rest). On the right hand side, S represents the source terms for noise generation. Following Lighthill's acoustic analogy, a linearized wave equation neglects feedback of the turbulent flow on the wave propagation. This is valid for the far-field pressure, such that the pressure wave originates from a confined region of the configuration space in which S is nonzero. In such case, the wave equation is solvable by means of Green's functions. The ODT simulated velocity fields are the input for the calculation of the acoustic sources. We compare sound pressure levels obtained with the suggested method to those measured by Viswanathan [5]. Potential insights regarding the source terms and the modeling rationale in ODT will be discussed.

References

[1] Lighthill (1952), Proc. R. Soc. Lond. A 211, 564-587.
[2] Wang, He, Lv, Zhou, Fan, and Cen (2010), Flow Turbulence Combust. 84, 669-686.
[3] Sharma, Klein, and Schmidt (2022), Phys. Fluids 34, 085134.

[4] Lilley (2003), Int. J. Aeroacoustics 2(3-4), 241-254.
[5] Viswanathan, 13th AIAA/CEAS Aeroacoustics Conf. (28th AIAA Aeroacoustics Conf.), 2007.

Estimation of ODT-resolved acoustic sources in high Reynolds number turbulent jets

Sharma, Sparsh *(Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom; Chair of Numerical Fluid and Gas Dynamics, BTU Cottbus-Senftenberg, Germany)*
Ayton, Lorna *(Department of Applied Mathematics and Theoretical Physics, University of Cambridge, United Kingdom)*
Klein, Marten *(Chair of Numerical Fluid and Gas Dynamics, BTU Cottbus-Senftenberg, Germany)*
Schmidt, Heiko *(Chair of Numerical Fluid and Gas Dynamics, BTU Cottbus-Senftenberg, Germany)*
12:20

This article discusses the use of one-dimensional turbulence (ODT) in predicting self-noise from a turbulent jet. ODT allows for the estimation of velocity fluctuations required for predicting self-noise. The study compares the axial profile of low-order fluctuation statistics of axial velocity fluctuations u' with experimental data from previous studies and finds reasonable agreement. The comparison also shows that the end of the potential core, which is a known source of noise, is well-described by ODT. Turbulent fluctuations govern the variability of the momentary extent of the potential core, rendering the high-fidelity modeling of such fluctuations a crucial aspect for jet noise applications.

The study also examines the self-similarity of a turbulent jet and shows that it becomes self-similar approximately 100 radii downstream of the nozzle. The self-similar plateau for round jets reaches its maximum value at $x=x_c+4r_0$. At this location, the ratio of the root-mean-square of the velocity fluctuation to the mean velocity is 0.160 for ODT, which matches well with reference large eddy simulation data. The turbulence intensity increase along the jet axis is dependent on the Reynolds number, which partly explains differences between reference data.

The article further discusses the use of Lighthill's equation, which requires the time history of fluctuating part of the Reynolds stress from ODT. The advection on the one-dimensional domain in ODT is implemented as a sequence of instantaneous events, making the flux interpretation of
quantities such as the Reynolds stress component $< u'_1 u'_2 >$ is not applicable if these quantities are computed conventionally in ODT directly from the velocity components. To evaluate Reynolds stresses and other advective fluxes in ODT, eddy-induced fluxes during simulated realizations are monitored to ensure the conservation laws and balance equations are satisfied exactly. Finally, the individual influence of each term in the Reynolds stress on the far-field noise is important to understand.

In conclusion, the study shows that ODT is a promising tool for predicting self-noise from turbulent jets. The comparison with previous studies demonstrates the accuracy of ODT in describing the end of the potential core, which is a significant source of noise. The self-similarity of turbulent jets and the individual influence of each term in the Reynolds stress on

far-field noise are also important factors to consider in predicting self-noise. Overall, ODT provides a valuable tool in predicting self-noise from turbulent jets.

Vortex cusps

Elling, Volker *(Academia Sinica, Taipei, Taiwan)* 12:40

Vortex cusps are pairs of self-similar vortex sheets with opposite circulation that merge in a cusp. Such solutions are observed in engineering flows, for example vortex sheets in Mach reflection at a solid wall. We present modelling and numerics of vortex cusps, calculate the cusp exponent and discuss possible rigorous existence proofs.

S13: Flow control

Organizer(s): **Grundmann, Sven** *(U Rostock)*
Kriegseis, Jochen *(KIT Karlsruhe)*

S13-01: Flow control

Date: May 30, 2023 13:30-16:10
Room: CHE/S91

Controlling shock-induced separation with air-jet vortex generators

Schreyer, Anne-Marie *(RWTH Aachen University, Germany)* 13:30

Shock-induced separation leads to highly unsteady flow fields and has strong detrimental effects on the aerodynamic behavior and performance of numerous aerospace-engineering applications. To reduce these effects, separation control is required. A very promising method uses rows of air-jet vortex generators (AJVGs), where small spanwise-inclined jets of air injected into the flow increase the momentum transfer within the boundary layer, and thus make it less prone to separation. A large number of parameters influences the control effectiveness of these devices, amongst them geometrical parameters, such as the orifice shape, orifice size, and injection-pipe length; flow parameters, including the injection pressure; and the array arrangement. The jet spacing within a control array and the injection pressure govern the degree of interactions between the turbulent structures induced by neighboring jets. Jet / jet interactions of medium strength enhance the control effectiveness of AJVGs, whereas strong interactions even have a detrimental effect. This control parameter is unique to air-jet vortex generators, as they are small enough for inter-device spacings allowing for favorable interactions - in contrast to the larger mechanical vortex generators.

An overview will be provided on the relevant control parameters and their respective influences, and the physical mechanisms and underlying flow dynamics governing the control effect of AJVGs will be presented. For these purposes, results from recent experimental and numerical studies will be discussed. In the trisonic wind-tunnel facility at RWTH Aachen University, we have carried out experimental analyses on AJVG control of a compression-ramp interaction with large-scale separation. For these experiments, a 24-degree compression ramp was installed on a flat-plate model; interchangeable rows of AJVGs with different properties were used for control purposes. The turbulent flow at a Mach number of M=2.5 was investigated with particle-image velocimetry and flow-visualization techniques. In addition, we performed large-eddy simulations of rows of AJVGs, as well as of individual devices, in a turbulent boundary layer at the same conditions as studied experimentally to analyze the details of the forming jet-in-crossflow configurations. A joint analysis of this rich experimental-numerical data set with statistical methods and modal analysis with dynamic-mode decomposition, amongst other techniques, allows an in-depth interpretation of observed flow phenomena and control effects, as well as the explanation of relevant control mechanisms.

Design Optimization of Three-dimensional Geometry of a Micro Horizontal Axis Wind Turbine Blade Using the Response Surface Method

Bekkai, Riyadh *(Echahid Cheikh Larbi Tebessi University, Algeria)*
Laouar, Roudouane *(Echahid Cheikh Larbi Tebessi University, Algeria)*
Mdouki, Ramzi *(Echahid Cheikh Larbi Tebessi University, Algeria)*
14:10

Wind turbine systems are considered among the most important renewable energy resource in the word. In order to obtain a optimal design, it is essential to understand the design and identify the best values of parameters affecting the blades of the wind turbine. The objective of this work is to re-design three-dimensional geometry of a micro-horizontal-axis wind turbine blade (HAWT). The focus is on the performance analysis and flow visualization of the baseline blade and the optimized one using CFD analyzer. The use of the built-in CFD optimization tools can shorten the design optimization cycle time, on other hand, the CFD analyzer allows a detailed topology of the 3D flow and predict the flow separation phenomenon on the blade surfaces. The goal driven optimization methodology (GDO) is used in order to obtain the optimal blade design. This methodology is based on the MOGA method (Multi-Objective-Genetic Algorithm), which consists of the entering of the input parameters in the design of exploration algorithm based on screening method, and then extracting the relationships between input and output parameters. Moreover, multi-curves correlations have been built to obtain the response surface, and finally the estimated optimal input and output parameters are used to build the optimal blade. The input parameters are chosen based on the two most important factors affecting the blade efficiency, chord length and twist angle distributions, and the performance is also monitored based on the torque values. CFD analyzer results are compared with ones of the open-source software (Qblade) for different tip speed ratio values

Control of the formation of the boundary layer over a surface with a cavity

Voropaiev, Gennadii *(Institute of Hydromechanics, Ukraine)*
Rozumnyuk, Nataliya *(Institute of Hydromechanics, Ukraine)*
Baskova, Oleksandra *(Institute of Hydromechanics, Ukraine)*
14:30

Any functionally necessary changes in the quality or shape of a streamlined surface are going to affect the hydrodynamic characteristics of bodies moving in a continuous medium, from a slight increase in drag to a complete loss of controllability of moving bodies caused by non-stationary separation generated by a change in the shape of the surface. Those problems have been well studied, and there is a sufficient amount of reference material, based on which it is possible to evaluate the influence of inhomogeneity on a streamlined surface in a given range of Reynolds and Mach numbers. However, when the characteristic dimensions of the necessary inhomogeneities on the streamlined surface exceed the recommended parameters, and the inhomogeneities become a source of large-scale non-stationary vortex formations, it is required to solve the problem of finding an external influence that could eliminate the conditions for the appearance of these structures or regulate their intensity and frequency of occurrence.

Including the problem of the formation of vortex flows in cavities and the conditions for their destruction. When the ratio of cavity width to the displacement thickness of the boundary

layer (θ) impinging on the cavity exceeds 50, the cavity becomes a source of throwing of vortical formations into the flow, which scale is determined by the cavity depth.

This paper presents the results of a numerical study of the vortical structure in a rectangular cavity. Depending on the Reynolds number, the numerical modeling was performed based on solving the Navier-Stokes equations, or RANS using the Reynolds stress transport model of turbulence, both in two-dimensional and three-dimensional formulations. The numerical results correlate with the experimental results, both in terms of the frequency parameters of vortex shedding from the cavity when the specified parameter is exceeded, and the essential characteristics of the cavity drag.

Based on the results of numerical modeling, a method is proposed for controlling the structure of the vortex flow in the cavity and the intensity of the cavity vortex wake using a low-intensity pulsating blowing (from the cavity bottom). First, the value of the blowing frequency is determined, starting from which, for a given Reynolds number, a stable circulation flow in the cavity is restored, the cavity drag decreases, and its low-frequency effect on the boundary layer in the wake behind the cavity is practically absent.

Surrogate-based optimization for active drag reduction of turbulent boundary layer flows

Hübenthal, Fabian *(RWTH Aachen University, Germany)*
Albers, Marian *(RWTH Aachen University, Germany)*
Meinke, Matthias *(RWTH Aachen University, Germany)*
Schröder, Wolfgang *(RWTH Aachen University, Germany)*

14:50

A significant portion of the energy demand and associated greenhouse gas emissions originate from the transportation sector, with air travel and high-speed rail accounting for a substantial share. Since fuel-burning jet engines will remain the primary propulsion source for large civil aircraft for decades to come and rising energy costs pose an economic challenge for high-speed trains, reducing energy demand and costs requires aerodynamic improvements. For that purpose, the active drag reduction technique of spanwise traveling transversal surface waves to manipulate the near-wall turbulent boundary layer to reduce viscous drag is analyzed, which is less well studied than passive techniques. From an optimization perspective, given the flow conditions, e.g., specified by the Reynolds and Mach numbers, the goal is to choose the non-dimensional actuation parameters, i.e., amplitude, wavelength and period, such that the objectives of drag reduction and net power savings are optimized while other aerodynamic properties, such as the lift-to-drag ratio for airfoils, are neutrally or even positively affected. The partially conflicting objectives drag reduction and net power savings are evaluated using wall-resolved Large-Eddy Simulations (LESs) based on the body-fitted deformable structured grid-based finite volume solver part of the in-house solver framework m-AIA. Since LESs at High-Performance Computing (HPC) scale are computationally expensive and the design space of choices is too vast to be sufficiently investigated by grid search methods, two surrogate-based optimization strategies are currently selected to guide the determination of optimal actuation settings. In the first previous study, precomputed LES data of a flat plate approximation are smoothly interpolated using Support Vector Regression (SVR),

focusing on the dependence of the drag reduction on the actuation parameters. The resulting SVR model is used to identify the a-priori assumed ridgeline, i.e., the curve connecting the wavelength-parameterized optima locations, by applying symbolic regression. Based on the prior knowledge of self-similarity and Tomiyama-Fukagata scaling for the local skin friction coefficient, the ridgeline is extrapolated 66% beyond the initial wavelength range, revealing an unexplored and numerically validated optimization potential. This second study focuses on extending the previous optimization pipeline using an SVR-based ridgeline surrogate to an automated optimization loop that addresses the exploration-exploitation trade-off using Bayesian Optimization (BO) with Gaussian Process (GP) prior as a surrogate. The prior knowledge utilized for and obtained by the SVR-based ridgeline optimization is incorporated into the GP prior to efficiently guide the optimization of the actuation parameters in a closed-loop.

Performance estimation of small-scale horizontal axis wind turbine blade

Laouar, Roudouane *(Larbi Tebessi University, Algeria)* 15:10
Bekkai, Riyadh *(Larbi Tebessi University, Algeria)*
Mdouki, Ramzi *(Larbi Tebessi University, Algeria)*

A wind turbine is a device that extracts kinetic energy from the wind and converts it into mechanical energy. This extracted energy is influenced by the geometry of the rotor blades. Determining the aerodynamic optimum blade shape, is one of the main tasks of the wind turbine designer.

The goal of this work is to design and optimize the performance of a small Horizontal-Axis-Wind-Turbine to achieve the best power coefficient (CP) at a low wind speed (5-10 m/s). Different airfoils were used and compared to get the optimized configuration.

A parametric numerical study and Simulation was conducted, in order to determine the optimum distribution of chord length and twist angle along the length of the blade at given windspeed. The QBlade software based on the blade element momentum (BEM) theory was used. The numerical simulation is carried out by Ansys Fluent.

The results of the two approaches were compared for different tip speed ratio values and a good agreement between CFD and BEM results was found.

S14: Applied analysis

Organizer(s): **Thomas, Marita** *(WIAS Berlin)*
Neukamm, Stefan *(TU Dresden)*
Schmidtchen, Markus *(TU Dresden)*

S14-01: Applied analysis

Date: May 30, 2023 13:30-16:10
Room: POT/51

Sedimentation of Particles with Very Small Inertia in Stokes Flows

Höfer, Richard *(Universität Regensburg, Germany)* 13:30
Schubert, Richard *(Universität Bonn, Germany)*

We consider the sedimentation of N spherical particles with identical small radii R_N to 0 in a Stokes flow in R^3. The particles satisfy a no-slip boundary condition and are subject to constant gravity. The dynamics of the particles is modeled by Newton's law but with very small particle inertia ϵ_N to 0 as N tends to infinity. We show that in this limit and under a mean-field scaling, the particle evolution is approximated in the 2-Wasserstein distance to order $O(\epsilon)$ by the transport-Stokes system which has been derived previously as the mean-field limit of inertialess particles. In particular this justifies to neglect the particle inertia in the microscopic system, which is a typical modelling assumption in this and related contexts. Moreover, in a monokinetic setting, we show that the particle evolution is approximated in the 2-Wasserstein with a smaller error by the Vlasov-Stokes eqautions that takes into account the (small) particle inertia.

An existence theory for solitary waves on a ferrofluid jet

Groves, Mark David *(Saarland University, Germany)* 13:50
Nilsson, Dag *(Lund University, Sweden)*
Schütz, Leon *(Weierstraß-Institute for Applied Analysis and Stochastics, Germany)*

We prove the existence of several families of axisymmetric solitary waves on the surface of an otherwise cylindrical ferrofluid jet surrounding a stationary wire. The ferrofluid flow which is assumed to be inviscid, incompressible and irrotational, is subject to a magnetic field which is generated by a current flowing along the wire. In the previous literature the ferrofluid waves are modelled by formally approximating the governing equations by a Korteweg-de Vries equation (strong surface tension) or by a nonlinear Schrödinger equation (weak surface tension). Using spatial dynamics methods, the formal approximations were proven rigorously by Groves & Nilsson (2018). In this work we directly use the Zakharov-Craig-Sulem formulation of the ferrofluid problem where we reformulate the governing equations via a Dirichlet-Neumann operator and solve the reduced equations using fixed-point arguments.

Coagulation equations for non-spherical clusters

Cristian, Iulia *(University of Bonn, Germany)*
Velázquez, Juan J. L. *(University of Bonn, Germany)* 14:10

We investigate the long-time asymptotics of a coagulation model which describes the evolution of a system of particles characterized by their volume and surface area. The aggregation mechanism takes place in two stages: collision and fusion of particles. We assume the coagulation kernel has a weak dependence on the area variable. We discover that the long-time analysis of the system is strictly related to the chosen fusion rate. We prove existence of self-similar profiles for some choices of the functions describing the fusion rate for which the particles have a shape that is close to spherical. On the other hand, for other fusion mechanisms, we show that the particle distribution describes a system of ramified-like particles. Lastly, we discuss how we are able to recover the standard coagulation equation in the case of fast fusion.

The diffusion equilibrium approximation of the stationary radiative transfer equation.

Dematté, Elena *(University of Bonn, Germany)*
Velázquez, Juan José *(University of Bonn, Germany)* 14:30

We study the situation where a body interacts with radiation only. We consider the boundary value problem for the stationary radiative transfer equation under the assumption of local thermodynamic equilibrium. We study the diffusion equilibrium approximation where there is no scattering. We consider the constant absorption coefficient and the limit when the optical depth tends to zero, i.e. the absorption coefficient tends to infinity. We show that the function u of the temperature defined by the Stefan-Boltzmann law $u=T^4$ solves in the limit a Laplace equation where the boundary value depends explicitly on the original boundary condition. We combine the method of matched asymptotics expansions and the analysis of non-local integral operators.

Convergence to self-similar profiles in reaction-diffusion systems

Mielke, Alexander *(Weierstraß-Institut Berlin, Germany; Humboldt Universität zu Berlin, Germany)*
Schindler, Stefanie *(Weierstraß-Institut Berlin, Germany)* 14:50

In this talk, we consider a coupled system of nonlinear reaction-diffusion equations on the entire real line, which present the concentration change of two diffusing species that interact through a single reversible reaction according to the mass-action law. By assuming that the solutions are in equilibria at infinity, we investigate the long-time behavior. Using parabolic scaling variables, we show that the solutions converge to constant profiles. In the original variables, these profiles correspond to asymptotically self-similar behavior describing the diffusive mixing of the different states at infinity. The idea is to use entropy estimates with the relative Boltzmann entropy functional. It is a standard approach for reaction-diffusion systems of mass-action type on bounded domains. While this method is well-studied on bounded domains, things become more complicated on the whole space.

An effective bulk-surface thermistor model for large-area organic light-emitting diodes

Glitzky, Annegret *(Weierstrass Institute (WIAS), Germany)* 15:10

We motivate a bulk-surface thermistor model describing the electrothermal behavior of large-area thin-film organic light-emitting diodes (OLEDs). This effective model was derived from a p(x)-Laplace thermistor model by dimension reduction and consists of the heat equation in the three-dimensional glass substrate and two semi-linear equations for the current flow through the electrodes coupled to algebraic equations for the continuity of the electrical fluxes through the organic layers. The electrical problem is formulated on the surface of the glass substrate where the OLED is mounted. The source term in the heat equation describes the Joule heating and is hence concentrated on the part of the boundary where the current-flow equation is posed. The existence of weak solutions to this effective system is proved via Schauder's fixed-point theorem. Since the heat source has a priori only pure integrability, the concept of entropy solutions is used. This is joint work with Matthias Liero from WIAS Berlin.

Existence results for ferromagnetic elastomers

Bresciani, Marco *(FAU Erlangen-Nürnberg)*
Friedrich, Manuel *(FAU Erlangen-Nürnberg)*
Mora-Corral, Carlos *(Universidad Autónoma de Madrid)* 15:30

We study a variational model for ferromagnetic elastomers featuring a mixed Eulerian-Lagrangian formulation. The magnetic variable is defined on the deformed configuration in the actual space and the saturation constraint involves the Jacobian determinant of deformations. We prove the existence of equilibrium configurations, first by restricting ourselves to purely elastic materials. Subsequently, we address the case of soft materials possibly subject to cavitation.

S14-02: Applied analysis

Date: May 31, 2023 08:30-09:30
Room: POT/51

A Nonlocal Maximum Principle

Huschens, Julia *(Trier University, Germany)* 08:30

Throughout the last years, increased attention has been devoted to the investigation of nonlocal models in which points separated by a non-vanishing distance interact with each other. In this talk, we present a weak maximum principle for nonlocal boundary value problems and point out a possible application.

Maximum principle for fourth-order hyperbolic equations with applications.

Buryachenko, Kateryna *(Vasyl' Stus Donetsk National University, Ukraine)* 08:50

We establish maximum principle and study the qualitative properties of weak solutions of Cauchy problem for fourth-order linear hyperbolic equations in plane domains. Most of these equations serve as mathematical models of many physical processes and attract the interest of researchers. The most famous of them include elasticity beam equations (Timoshenko beam equations with and without internal damping), the short laser pulse equation, equations which describe the structures that are subjected to moving loads, equation of Euler-Bernoulli beam resting on two-parameter Pasternak foundation and subjected to a moving load or mass and others. The main novelty is the maximum principle for fourth-order linear hyperbolic equations in plane domains with further application to the problems of well-possedness to Cauchy problem and solution behavior in physical interpretation. We use notion of L-traces and develop the new effective methods for investigation the qualitative properties of solutions of Cauchy problem with initial (boundary) conditions of weak regularity for the two dimensional linear fourth-order hyperbolic equations (weak maximum principle, energetic estimates, operator methods, moment problem). These results are applied to describe the processes of beam elasticity (with and without internal damping), short laser pulse, structures are subjected to moving loads and others.

Regional problem

Vu, Michael *(Trier University, Germany)* 09:10

In nonlocal models points separated by a non-vanishing distance interact with each other. Therefore, domains separated by a non-vanishing distance can be coupled in these models. In this talk, we reformulate a nonlocal Neumann problem and we, moreover, consider parabolic nonlocal Neumann equations.

S14-03: Applied analysis

Date: May 31, 2023 14:00-16:00
Room: POT/51

Universality of the magnetisation ripple – variational methods for a singular stochastic PDE

Ignat, Radu *(Institut de Mathématiques de Toulouse & Institut Universitaire de France)*
Otto, Felix *(Max Planck Institute for Mathematics in the Sciences Leipzig)*
Ried, Tobias *(Max Planck Institute for Mathematics in the Sciences Leipzig)*
Tsatsoulis, Pavlos *(Bielefeld University)*

14:00

The magnetisation ripple is a microstructure formed in thin ferromagnetic films. It can be described by minimisers of a non-convex energy functional leading to a nonlocal and nonlinear elliptic stochastic PDE in two dimensions driven by white noise, which is singular. In this talk I want to describe how the universal character of the magnetisation ripple can be addressed using variational methods based on Γ-convergence. More precisely, universality holds in the class of (not necessarily Gaussian) approximations to white noise satisfying the spectral gap inequality, which allows us to obtain sharp stochastic estimates.

Variational models for pattern formation in biomembranes: A Gamma-convergence result

Ginster, Janusz *(Humboldt-Universität zu Berlin, Germany)*
Hayrapetyan, Gurgen *(Columbia University, New York, NY)*
Pešić, Anastasija *(Humboldt-Universität zu Berlin, Germany)*
Zwicknagl, Barbara *(Humboldt-Universität zu Berlin, Germany)*

14:40

Biological membranes are thin structures that are composed of various components. The different components often form microdomains, called lipid rafts, that are arranged in complex patterns. To explain this pattern formation, variational models based on Cahn-Hilliard type energies have been introduced that couple the local composition of the membrane to its local curvature, which makes the resulting functionals nonlocal.

The main focus of this talk lies on the derivation of the Gamma-limit in a certain parameter regime where the limiting functional turns out to be of perimeter-type. As a main novelty, we will present a technique to include Neumann-boundary conditions in the construction of a recovery sequence.

A homogenized bending theory for prestrained plates

Padilla-Garza, David *(TU Dresden, Germany)*
Neukamm, Stefan *(TU Dresden, Germany)*
Boehnlein, Klaus *(TU Dresden, Germany)*
Sander, Oliver *(TU Dresden, Germany)*

15:00

Nonlinear plate theory described the energy of an incompressible and inextensible thin elastic sheet. In this work, we show a general rigorous derivation of a generalization of such a model for non-euclidean plates with microheterogeneous structures. We also analyze the limiting energy in some examples and discover interesting and counter-intuitive phenomena.

One-dimensional viscoelastic von Kármán theories

Machill, Lennart *(WWU Münster, Germany)*
Friedrich, Manuel *(FAU Erlangen-Nürnberg, Germany)* 15:20

A one-dimensional limit is derived from a three-dimensional Kelvin-Voigt model for thin-walled viscoelastic beams, in which the elastic and the viscous stress tensor comply with a frame-indifference principle. The limiting system of equations comprises stretching, bending, and twisting in both the elastic and viscous stress. It can be identified through a successive dimension reduction, passing from a 3D to a 2D-theory for von Kármán plates [Friedrich-Kružík '20], followed by a reduction from 2D to 1D for ribbons [Friedrich-Machill '22]. Additionally, it can also be derived by a simultaneous reduction from 3D to 1D. The arguments rely on the static Γ-convergence in [Freddi-Mora-Paroni '13], on the abstract theory of metric gradient flows, and on evolutionary Γ-convergence [Sandier-Serfaty '04].

A Gamma-convergence result for discrete elastic rods

Hounkpe, Coffi Aristide *(Albert-Ludwigs-Universität Freiburg, Germany)*
Dondl, Patrick W. *(Albert-Ludwigs-Universität Freiburg, Germany)*
Jesenko, Martin *(Univerza v Ljubljani)* 15:40

This work is motivated by the classical discrete elastic rod model by Audoly et al. We derive a discrete version of the Kirchhoff elastic energy for rods undergoing bending and torsion and prove Gamma-convergence to the continuous model. This discrete energy is given by the bending and torsion energy of an interpolating conforming polynomial curve and provides a simple formula for the bending energy depending on each discrete segment only on the angle and adjacent edge lengths. For the Liminf-inequality, we need to introduce penalty terms to ensure arc length parametrization in the limit. For the recovery sequence, a discretization with an equal euclidean distance between consecutive points is constructed. Particular care is taken to treat the interaction between bending and torsion by employing a discrete version of the Bishop frame.

S14-04: Applied analysis

Date: June 1, 2023 08:30-10:30
Room: POT/51

A nonlocal approach to cell migration in heterogeneous environments

Surulescu, Christina *(RPTU Kaiserslautern-Landau, Germany)* 08:30
Eckardt, Maria *(RPTU Kaiserslautern-Landau, Germany)*
Painter, Kevin *(Politecnico di Torino)*
Zhigun, Anna *(Queen's University Belfast)*

Increasing experimental evidence suggests that cells are able to sense physical and chemical cues in their environment, up to several cell diameters around their current position. This motivated the development of continuous mathematical models which account for various types of (spatial) nonlocalities, most of them addressing cell-cell and/or cell-matrix adhesions. They can be classified according, e.g., to the type of featured nonlocality. We present a modeling approach with spatial nonlocality in the drift described via integral operators applied directly to gradients of signal-dependent quantities and being able to handle hapto- and chemotactic behavior in a unified manner. For a shrinking radius of the cell sensing region, the nonlocal formulation converges to a local reaction-diffusion-taxis setting. Numerical simulations in 1D are used to illustrate the results and compare to previous models. This is joint work with Maria Eckardt (RPTU Kaiserslautern-Landau), Kevin Painter (Politecnico di Torino), and Anna Zhigun (Queen's Univ. Belfast).

Two-phase flows with bulk-surface interaction: A Navier–Stokes–Cahn–Hilliard model with dynamic boundary conditions

Knopf, Patrik *(Universität Regensburg, Germany)* 09:10
Giorgini, Andrea *(Politecnico di Milano, Italy)*

We consider a novel thermodynamically consistent Navier-Stokes-Cahn-Hilliard system with dynamic boundary conditions. This model describes the motion of viscous incompressible binary fluids with different densities. In contrast to previous models in the literature, our new model allows for surface diffusion, a variable contact angle between the diffuse interface and the boundary, and mass transfer between bulk and surface. In particular, this transfer of material is subject to a mass conservation law including a bulk and a surface contribution. The model derivation is carried out by means of local energy dissipation laws and the Lagrange multiplier approach. In the case of fluids with matched densities, we show the existence of global weak solutions in two and three dimensions as well as the uniqueness of weak solutions in two dimensions.

Optimal distributed control for a non-local viscous diffuse interface tumour growth model

Fornoni, Matteo *(University of Pavia, Italy)* 09:30
Rocca, Elisabetta *(University of Pavia, Italy)*

We consider a non-local and viscous variant of a diffuse interface model for tumour growth proposed by Hawkins-Daarud et al. (2012). This model consists of a non-local viscous Cahn-

Hilliard equation for the tumour phase parameter, coupled to a reaction-diffusion equation for the nutrient. Due to the viscous regularisation, we can take into account both singular and regular potentials, as well as the effect of chemotaxis, even in three spatial dimensions. First, we prove the weak and strong well-posedness of the system of partial differential equations, by adapting the arguments of Frigeri et al. (2017) and Scarpa et al. (2021). In particular, due to a different reaction term, we are able to improve the regularity results found previously, without needing additional regularisations. Next, we introduce a distributed optimal control problem, where the objective is to find an optimal therapy that could lead the tumour to a desired final configuration. Regarding the treatments, we take into account both radiotherapies and chemotherapies. In this setting, we prove the existence of optimal controls and then, by studying the differentiability of the control-to-state operator and the adjoint system, we recover the first-order necessary optimality conditions.

On a diffuse interface model for incompressible viscoelastic two-phase flows

Liu, Yadong *(Universität Regensburg, Germany)*
Trautwein, Dennis *(Universität Regensburg, Germany)*
09:50

This talk concerns a diffuse interface model for the flow of two incompressible viscoelastic fluids in a bounded domain. More specifically, the fluids are assumed to be macroscopically immiscible, but with a small transition region, where the two components are partially mixed. Considering the elasticity of both components, one ends up with a coupled Oldroyd-B/Cahn-Hilliard type system, which describes the behavior of two-phase viscoelastic fluids. We prove the existence of weak solutions to the system in two dimensions for general (unmatched) mass densities, variable viscosities, different shear moduli, and a class of physically relevant and singular free energy densities that guarantee that the order parameter stays in the physically reasonable interval. The proof relies on a combination of a novel regularization of the original system and a new hybrid implicit time discretization for the regularized system together with the analysis of an Oldroyd-B type equation. This is joint work with Dennis Trautwein (Universität Regensburg)

Existence and approximation of a viscoelastic Cahn–Hilliard model for tumour growth

Trautwein, Dennis *(Universität Regensburg, Germany)*
Garcke, Harald *(Universität Regensburg, Germany)*
10:10

In this talk, we present a phase-field model for tumour growth, where a diffuse interface is separating a tumour from the surrounding host tissue. In our model, we include biological effects like chemotaxis and transport processes by an internal velocity field. We include viscoelastic effects with a general Oldroyd-B type description with stress relaxation and stress generation by growth. The main analytical result is the existence of weak solutions in a specific setting. The idea behind the proof is a numerical approximation of the model with a fully-practical, stable and converging discrete scheme, which preserves the physical properties of the model. Finally, we illustrate properties of solutions with the help of numerical simulations.

S14-05: Applied analysis

Date: June 1, 2023 16:00-19:00
Room: POT/51

Nonlocal cross-interaction systems on graphs

Pietschmann, Jan-Frederik *(Universität Augsburg)* 16:00
Heinze, Georg *(Universität Augsburg)*
Schmidtchen, Markus *(Technische Universität Dresden)*

The rigorous understanding of evolution equations as gradient flows on graphs has gained much interest recently. We review the recent results of Esposito et. al. (2021), which are then extended by studying the evolution of a system of two species with nonlinear mobility with nonlocal interactions. We provide a rigorous interpretation of the interaction system as a gradient flow in a Finslerian setting. Weakening the notion of Minkowski norm and nonlocal gradient, in the spirit of Agueh (2011), the geometric interpretations and the analysis are carried over to p-Wasserstein-like distances. We also explore the dynamical behaviour and energetic properties of the mode, complemented by numerical examples.

Regularisation and separation for evolving surface Cahn-Hilliard equations

Caetano, Diogo *(University of Warwick, UK)* 16:40
Elliott, Charles M. *(University of Warwick, UK)*
Grasselli, Maurizio *(Politecnico di Milano, Italy)*
Poiatti, Andrea *(Politecnico di Milano, Italy)*

In this talk I would like to present some recent results about the mathematical analysis of phase field models on evolving surfaces, obtained in collaboration with Maurizio Grasselli, Charles M. Elliott and Diogo Caetano. We analyze the Cahn-Hilliard equation (with logarithmic potential) on an evolving two-dimensional surface embedded in $\mathbf{R}^3$, whose evolution is assumed to be given a priori, and study two models, derived from balance laws for an order parameter with an associated Cahn-Hilliard energy functional. We continue the analysis of [1], in which the well-posedness of weak solutions is proven, by first showing the instantaneous regularization property of weak solutions. The proof is carried out in a Galerkin approximation setting, suitably tuned to take into account the evolution of the surface. Exploiting this result, by adapting the standard techniques for stationary bounded domains to the case of an evolving two-dimensional surface, we are able to show the validity of the instantaneous strict separation property, i.e., we prove that any weak solution stays instantaneously away from the pure states. This is essential to determine higher-order estimates. The aim of this work is to have a complete analysis of the Cahn-Hilliard equation on evolving surfaces with prescribed velocity, in order to be able to treat, in future contributions, the fully coupled system, where the evolution of the surface is itself part of the problem. Applications of these models can be found in the cell membrane phase separation, leading to the formation of lipid rafts, which have been linked to a wide range of cellular functions, from membrane trafficking to inter- and intracellular signaling.

References:
[1] Caetano, D., Elliott, C.M. (2021), Cahn-Hilliard Equations on an Evolving Surface, European J. Appl. Math. 32, 937-1000.

On the analysis of a class of cross-diffusion systems with Cahn-Hilliard effects

Cauvin-Vila, Jean *(CERMICS, Ecole des Ponts, INRIA, France)*
Davoli, Elisa *(TU Vienna, Austria)*
Ehrlacher, Virginie *(CERMICS, Ecole des Ponts, INRIA, France)*
Marino, Greta *(Universität Augsburg, Germany)*
Pietschmann, Jan-Frederik *(Universität Augsburg, Germany)*

17:00

Systems of partial differential equations with cross-diffusion have gained a lot of interest in recent years, and find applications in many areas such as the modeling of population dynamics of multiple species, cell sorting or chemotaxis-like applications, the predator-swarm model, and so on. On the other hand, the Cahn-Hilliard equation was initially developed to describe phase separation in a two components system (metallic, polymer, glassy components), where the unknown u= u(t,x) represents the concentration (volume or mass fraction) of one of the components.

In this talk we present a system that combines the two effects mentioned above, and models a multicomponent mixture in which only one species (that accounts for the void) does separate from the others. The interest for such a model stems from the fact that in many real world applications there exist multiphase systems where miscible entities may coexist in one single phase of the system.

After an introduction of the model, we will present an existence result of weak solutions to the system, and then we will provide an analysis of its stationary solutions as well as the large-time asymptotics. If time allows, we will conclude with some comments on the nonlocal Cahn-Hilliard contribution.

On a Thermodynamically Consistent Electro-Energy-Reaction-Diffusion System

Kniely, Michael *(WIAS Berlin, Germany)*
Mielke, Alexander *(WIAS Berlin, Germany)*

17:20

We consider a thermodynamically correct formulation of reaction-diffusion systems modeling the evolution of a mixture of charged species. Our model consists of a gradient flow system in Onsager form for the concentrations and the internal energy, while the electrostatic potential is determined via Poisson's equation. The talk will first focus on the structure of the Onsager operator, its dependence on the electrostatic potential, and the validity of fundamental conservation laws. We shall also address similarities and differences compared to other temperature-dependent semiconductor-type models concerning, e.g., the choice of independent variables, employed entropy functionals, and admissible mobility matrices. Funded by an FWF fellowship, it is one of the goals of this project to construct global (weak or renormalized)

solutions to our electro-energy-reaction-diffusion system. Preliminary results in an appropriate framework will be presented, while open problems shall be discussed as well. This project is ongoing work together with Alexander Mielke.

Excluded volume and order in systems of Brownian needles

Bruna, Maria *(University of Cambridge, United Kingdom)*
Chapman, Jon *(University of Oxford, United Kingdom)*
Schmidtchen, Markus *(Technische Universität Dresden, Germany)*

17:40

We consider a system of nonoverlapping Brownian needles in two dimensions. Unlike point particles, the needles' size and shape influence the system's evolution. We explore the effects of excluded volume and anisotropy at the population level. Since needles exclude less volume if aligned, can excluded-volume effects alone induce order in the system? Starting from the stochastic particle system, we derive a nonlocal nonlinear partial differential equation for the population density using the methods of matched asymptotic expansions and conformal mapping. Finally, we show some numerical simulations and two model reductions.

A model for lime consolidation of porous solids

Detmann, Bettina *(Universität Duisburg-Essen, Germany)*
Gavioli, Chiara *(Technische Universität Wien, Austria)*
Krejčí, Pavel *(Czech Technical University, Czech Republic)*
Lamač, Jan *(Czech Technical University, Czech Republic)*
Namlyeyeva, Yuliya *(Czech Technical University, Czech Republic)*

18:00

We present the first mathematical 3D model describing the process of filling the pores of a building material with a water-lime-mixture, with the goal to improve the consistency of the porous solid. Chemical reactions produce calcium carbonate which glues the solid particles together at some distance from the boundary and strengthens the whole structure. The model consists of a reaction-diffusion system with a nonlinear non-smooth boundary condition, coupled with the mass balance equations for the chemical reaction. The main result consists in proving that the system has a solution for each initial data from a physically relevant class. A 1D numerical test shows a qualitative agreement with experimental observations.

S14-06: Applied analysis

Date: June 2, 2023 08:30-10:30
Room: POT/51

Sharp Interface Limit of a Navier-Stokes/Allen-Cahn system with vanishing mobility via rigorous asymptotic expansions

Abels, Helmut *(University Regensburg, Germany)* 08:30
Fei, Mingwen *(Anhui Normal University, Wuhu, China)*
Moser, Maximilian *(Institute of Science and Technology Austria, Klosterneuburg, Austria)*

We consider the sharp interface limit of a Navier-Stokes/Allen-Cahn system, when a parameter ϵ>0 that is proportional to the thickness of the diffuse interface tends to zero, in a two dimensional bounded domain. In dependence on the mobility coefficient in the Allen-Cahn equation in dependence on ϵ>0 different limit systems or non-convergence can occur. In the case that the mobility is proportional to the square root of ϵ solutions convergence to a solutions of a classical sharp interface model on short times for well-prepared and sufficiently smooth initial data. To this end we construct a suitable approximation of the solution of the Navier-Stokes/Allen-Cahn system using an expansion with half-integer powers of ϵ and suitable solutions of a linearized limit system. Then the difference of approximate and exact solution is estimated with the aid of a suitable spectral estimate of the linearized Allen-Cahn operator. This is a joint work with Mingwen Fei (Anhui Normal University, China), and Maximilian Moser (ISTA Klosterneuburg, Austria).

Sharp interface limit via relative entropy: Navier-Stokes/Allen Cahn system with vanishing mobility

Moser, Maximilian *(Institute of Science and Technology Austria (ISTA), Austria)* 08:50
Abels, Helmut *(University of Regensburg)*
Fischer, Julian *(Institute of Science and Technology Austria (ISTA), Austria)*

In this talk we consider the sharp interface limit of a Navier-Stokes/Allen Cahn equation in a bounded smooth domain in two dimensions when the small parameter ϵ>0 related to the thickness of the diffuse interface is sent to zero. The mobility in the Allen-Cahn equation is scaled in such a way that it converges to zero polynomially and less than quadratic with repect to ϵ. The limit problem is given by the classical two-phase Navier-Stokes-system with surface tension and we show convergence for well-prepared initial data and for small times such that a strong solution to the limit problem exists. The approach is via the relative entropy method, i.e. one shows a Gronwall-type estimate for suitable energy functionals that control the error between the solution to the diffuse and sharp interface systems in a suitable way. This is joint work with H. Abels (Univ. of Regensburg) and J. Fischer (IST Austria).

Schemes for approximating solutions of a rate-independent phase field damage model

Boddin, Samira *(University of Kassel, Germany)* 09:10
Knees, Dorothee *(University of Kassel, Germany)*

In this talk we consider a rate-independent phase field damage model describing the evolution of cracks in quasi-brittle materials. The nonconvexity of the energy functional within this model is challenging from the analytical as well as the computational point of view. In the rate-independent setting it may lead to a discontinuous evolution in time.

Several solution concepts for rate-independent systems allowing for jumps in time have been developed and in general they are not equivalent. The most prominent ones are the concept of (global) energetic solutions (GES) and the concept of balanced viscosity (BV) solutions. While the former is based on global energy minimization and tends to jump across energy barriers, the latter reflects local force balances in a better way and thus will be focused. A promising scheme for approximating BV solutions was introduced in [EM]. It combines local minimization with a time-adaptive strategy to resolve jumps rather accurately.

Another commonly applied strategy of approximating solutions, which is not analytically motivated, is alternate minimization (AM). Due to the fact that the energy functional of the damage model is at least separately convex with respect to the displacement field and the phase field variable, this strategy shows numerically good performance. However, solutions constructed like this can generally not be assigned to one of the solution concepts mentioned above.

In the joint work [BRKM] the time-adaptive scheme for approximating BV solutions from [EM] was combined with the AM strategy in order to make it applicable for the damage model. Convergence to BV solutions was shown. Moreover, first numerical experiments suggest that there is no essential difference in the approximate solutions generated by pure AM and by the combined scheme.

Within this talk the combined scheme from [BRKM] will be introduced. Afterwards the question, whether the combined scheme and pure AM essentially give the same solutions, will be investigated. Therefore finite-dimensional examples - not only separately convex, having in mind models with more complex structures - are considered.

[BRKM] S. Boddin, F. Rörentrop, D. Knees, J. Mosler. Approximation of balanced viscosity solutions of a rate-independent damage model by combining alternate minimization with a local minimization algorithm. https://arxiv.org/abs/2211.12940, 2022.
[EM] M. A. Efendiev and A. Mielke. On the rate-independent limit of systems with dry friction and small viscosity. *Journal of Convex Analysis*, 13(1):151-167, 2006.

A first-order formulation for dynamic phase-field fracture in viscoelastic materials

Thomas, Marita *(Free University of Berlin; Weierstrass Institute for Applied Analysis and Stochastics, Berlin)*
Tornquist, Sven *(Free University of Berlin)*
Weinberg, Kerstin *(University of Siegen)*
Wieners, Christian *(Karlsruhe Institute of Technology)*

09:30

We analyze a model for the description of fracture propagation in viscoelastic materials at small strains. For this, a phase-field approach is used to approximate the sharp crack surface and the crack evolution is damped with a quadratic dissipation potential. We concentrate on the wave aspect in the system and transform the elastic equation of motion into a first-order system of coupled equations. This is combined with a discontinuous Galerkin approach. Crack propagation and elasticity system are coupled in a nonlinear way, and the introduction of a non-smooth penalty term inhibits that material can heal. Based on this, a rigorous convergence analysis starting from a system fully discretized in space and time is provided.

On some generalizations of the notion of oscillatory sequence of functions and their applications

Raguz, Andrija *(Zagreb School of Economics and Management, Croatia)*

09:50

We consider Cahn-Hilliard functional with non-coercive two-well potential in one dimension. We address the problem of analyzing oscillation and concentration in its finite-energy sequences as small parameter epsilon tends to zero. In the case when a priori estimates in terms of classical norms are not available, we introduce some generalizations of the notion of oscillatory sequence of functions, and we apply those notions to analyze the aforementioned properties of finite-energy sequences.

Variational analysis of integral functionals involving nonlocal gradients on bounded domains

Schönberger, Hidde *(Katholische Universität Eichstätt-Ingolstadt, Germany)*
Cueto, Javier *(University of Nebraska-Lincoln, Nebraska)*
Kreisbeck, Carolin *(Katholische Universität Eichstätt-Ingolstadt, Germany)*

10:10

The center of interest in this talk are variational problems with integral functionals depending on special nonlocal gradients. The latter correspond to truncated versions of the Riesz fractional gradient, as introduced in [Bellido, Cueto & Mora-Corral 2022] along with the underlying function spaces. We contribute several new aspects to both the existence theory of these problems and the study of their asymptotic behavior. Our overall proof strategy builds on finding suitable translation operators that allow to switch between the three types of gradients: classical, fractional, and nonlocal. These provide useful technical tools for transferring results from one setting to the other.

Based on this approach, we show that quasiconvexity, which is the natural convexity notion in the classical - and as shown in [Kreisbeck & Schönberger 2022] also in the fractional - calculus of variations, gives a necessary and sufficient condition for the weak lower semicontinuity of

the nonlocal functionals as well. As a consequence of a general Gamma-convergence statement, we obtain relaxation and homogenization results. The analysis of the limiting behavior for varying fractional parameters yields, in particular, a rigorous localization with a classical local limit model.

S14-07: Applied analysis

Date: June 2, 2023 11:00-13:00
Room: POT/51

Optimal relaxation rates for the Mullins-Sekerka Evolution

Otto, Felix *(MPI MiS Leipzig, Germany)* 11:00
Schubert, Richard *(University of Bonn, Germany)*
Westdickenberg, Maria G. *(RWTH Aachen, Germany)*

We consider the evolution of a perturbation of the plane in three space dimensions by the Mullins-Sekerka law. This is a non-local third order geometric evolution that can be viewed as a nonlinear and non-convex gradient flow for the excess surface energy. Only assuming information on a characteristic dimensionless quantity, we prove that the surface becomes a graph, and that the energy converges with an optimal rate towards the ground state. This improves upon previous results both in terms of ambient dimension and rate of convergence.

Energy scaling laws for a variational model of epitaxial growth

Abel, Lukas *(HU Berlin, Germany)* 11:20
Ginster, Janusz *(HU Berlin, Germany)*
Zwicknagl, Barbara *(HU Berlin, Germany)*

Epitaxy is a special form of crystal growth and of great importance in modern technology. We consider a crystalline film that is deposited on a (rigid) substrate. The misfit between the crystal structure of the film and the substrate can lead to dislocations and can have an influence on the morphology of the film. Dislocations are topological defects of the crystallographic lattice.

In this talk we will study a variational model which takes dislocations into account. The focus of the talk will lie on the scaling laws for the minimial energy. The results indicate that in certain parameter regimes, the formation of dislocations is expected.

Truesdell's empirical inequalities and the coaxiality of stress and stretch

Voss, Jendrik *(TU Dortmund, Germany; University of Duisburg-Essen)* 11:40
Martin, Robert J. *(University of Duisburg-Essen)*
Neff, Patrizio *(University of Duisburg-Essen)*

Truesdell's empirical inequalities are considered essential in various fields of nonlinear elasticity. However, they are often used merely as a sufficient criterion for the semi-invertibility of the isotropic stress-strain relation, even though weaker and much less restricting constitutive requirements like the strict Baker-Ericksen inequalities are available for this purpose. We elaborate on the relations between such constitutive conditions, including a weakened version of the empirical inequalities, and their connection to bi-coaxiality and related matrix properties. In particular, we discuss a number of issues arising from the seemingly ubiquitous use of the phrase "X, Y have the same eigenvectors" when referring to commuting symmetric tensors X, Y.

Korn-Maxwell-Sobolev inequalities for general incompatibilities

Gmeineder, Franz *(University of Konstanz, Germany)*
Lewintan, Peter *(University of Duisburg-Essen, Germany)*
Neff, Patrizio *(University of Duisburg-Essen, Germany)*
12:00

We establish a family of coercive Korn-type inequalities for generalised incompatible fields in the superlinear growth regime under sharp criteria. This extends and unifies several previously known inequalities that are pivotal to the existence theory for a multitude of models in continuum mechanics in an optimal way. Especially, we obtain sharp generalisations of recently proved inequalities by the last two authors and Stefan Müller in the realm of incompatible Korn-type inequalities with conformally invariant dislocation energy. However, being applicable to higher order scenarios as well, our approach equally gives the first and sharp inequalities involving Kröner's incompability tensor inc.

Gel models for phase separation at finite strains

Schmeller, Leonie *(Weierstrass Institute, Germany)*
Thomas, Marita *(Weierstrass Institute, Germany; FU Berlin, Germany)*
12:20

Hydrogels are crosslinked polymer networks saturated in a liquid. During swelling and squeezing processes, they undergo enormous volume changes, which requires finite strain models for realistic considerations.

We analytically study a two-phase model for phase separation in a geometrically nonlinear elastic material. The coupled system of PDEs consists of a Cahn-Hilliard equation and a quasi-static mechanical force balance of the deforming gel. The phase field and the mechanics are coupled by a multiplicative decomposition of the deformation gradient, and time-dependent Dirichlet boundary conditions are imposed on the deformation field.

Based on an incremental scheme, we prove the existence of solutions in a suitable weak formulation. Using techniques from calculus of variations and nonlinear PDE theory, we obtain an existence result for the time-continuous problem under suitable assumptions.

This is joint work with Marita Thomas within the DFG Priority Program SPP 2171 *Dynamic Wetting of Flexible, Adaptive, and Switchable Substrates*, project #422786086 and within MATH$^+$ project AA2-9.

Analysis of poro-visco-elastic solids at finite strains

van Oosterhout, Willem *(Weierstrass Institute, Germany)*
Liero, Matthias *(Weierstrass Institute, Germany)*
12:40

Poro-visco-elastic solids are materials in which a species diffuses and contributes to their deformation. Taking the Biot model as starting point, we discuss the modelling of (large) deformations and diffusion processes in a physically consistent way, and show that under certain assumptions weak solutions exist. To model poro-visco-elastic materials, a free energy functional and dissipation potential are introduced. This energy functional has contributions both from the deformation gradient, i.e., an elastic contribution, and from a mixing term, which couples the deformation gradient and the concentration of the species. The dissipation potential features contributions for the viscous evolution and the diffusion process. In

particular, since the focus is on finite-strain elasticity, the diffusion equation has to be pulled back to the reference configuration. As the pulled-back mobility tensor depends nonlinearly on the deformation gradient, and the viscous stresses are frame-indifferent, it is analytically necessary to include the hyperstress as a higher-order regularization, which makes this a second order non-simple material. Another important property of the investigated model is that it allows for degenerate mobilities, which are more physically relevant; however, this greatly complicates the analysis, and requires an additional regularization step. This is in contrast to prior work, where only non-degenerate mobilities were considered. Still, under certain assumptions on the constitutive laws and the data, the existence of weak solutions to the coupled system is shown using variational methods. This is joint work with Matthias Liero (WIAS Berlin).

S14-08: Applied analysis

Date: June 2, 2023 16:00-18:00
Room: POT/51

Existence of Quasi-Static Crack Evolution for Atomistic Systems

Seutter, Joscha *(FAU Erlangen-Nürnberg, Germany)* 16:00
Friedrich, Manuel *(FAU Erlangen-Nürnberg, Germany)*
Badal, Rufat *(FAU Erlangen-Nürnberg, Germany)*

We consider atomistic systems consisting of interacting particles arranged in atomic lattices whose quasi-static evolution is driven by time-dependent boundary conditions. The interaction of the particles is modeled by classical interaction potentials where we implement a suitable irreversibility condition modeling the breaking of atomic bonding. This leads to a delay differential equation depending on the complete history of the deformation at previous times. We prove existence of solutions and provide numerical tests for the prediction of quasi-static crack growth in particle systems. We furthermore investigate the passage to the continuum limit by means of evolutionary Γ-convergence in the antiplane case.

Long-time dynamics and singular limits of transmission problems for elastic arch beams.

Fastovska, Tamara *(Humboldt Universität zu Berlin, Germany)* 16:20

We consider transmission problems describing dynamics of elastic arch beams consisting of two parts with different elastic properties. In particular, we investigate the Bresse system for arch beams with a structural damping terms in one or two equations . We show the existence of compact global attractors via showing the gradient structure and asymptotic smoothness of the dynamical system generated by the Bresse system. We also show that on finite time intervals, the system reduces to the transmission Timoshenko system when the arch curvature tends to zero and to the Kirhchoff system when the curvature and the shear moduli tend to zero and infinity respectively.

Well- and ill-posedness results on the hyperbolic Prandtl system in Gevrey-spaces

De Anna, Francesco *(University of Wuerzburg, Germany)* 16:40
Kortum, Joshua *(University of Wuerzburg, Germany)*
Scrobogna, Stefano *(Universita degli Studi di Trieste, Italy)*

The Prandtl equations attempt to model boundary layer formation in viscous fluid mechanics. From the mathematical point of view, the former system is of very unstable nature. Past investigations show that stable and regular solutions can only be expected for monotonic velocity profiles. In general, well-posedness only holds true in very regular function spaces, so-called Gevrey spaces, where the borderline regularity was recently set to the Gevrey-2 class. This talk addresses a hyperbolic variant of the Prandtl equations. In order to overcome the unphysical infinite-speed propagation in incompressible media, the use Cattaneo's law provides a physically-meaningful extension countering this fact. We extend the recent well-posedness findings on the classical Prandtl system to the linearised hyperbolic version resulting in a non-

trivial upgrade of regularity in the Gevrey-class 3. Further, we also hint at the optimality of these results with respect to ill-posedness in any larger space.

Energy-variational solutions for a class of hyperbolic conservation laws

Eiter, Thomas *(Weierstrass Institute for Applied Analysis and Stochastics, Germany)* 17:00
Lasarzik, Robert *(Weierstrass Institute for Applied Analysis and Stochastics, Germany)*

In this talk, the novel concept of energy-variational solutions is considered for a general class of hyperbolic conservation laws. This solution concept is derived from a variational formulation by introducing the weighted difference between the mechanical energy and an auxiliary variable representing the turbulent energy. If the weight is chosen in a suitable way, a general existence result can be derived via a time-discretization scheme based on a sequential minimization, and it does not require a spatial regularization. Moreover, the solution concept comes along with favorable properties like a weak-strong uniqueness principle and the convexity of solution sets. Finally, for the compressible and incompressible Euler equations, energy-variational solutions can be identified with dissipative weak solutions.

On Frictional Unilateral Contact in Finite Strain Elasticity

Gwinner, Joachim *(Universität der Bundeswehr München, Germany)* 17:20

Using the polyconvexity approach to nonlinear elasticity of J. Ball [1] to nonlinear elasticity we extend the work on unilateral contact in [2,3] to include frictional phenomena along the boundary of the elastic body. We combine penalization of the unilateral constraint with regularization of the friction term [4].

Some References

[1] Ball, J. M. (1976). Convexity conditions and existence theorems in nonlinear elasticity. Archive for rational mechanics and Analysis, 63(4), 337-403.

[2] Dvorsky, K., & Gwinner, J. (2009). Generalized convexity in nonlinear elasticity with applications to unilateral contact. Taiwanese Journal of Mathematics, 13(2B), 687-712.

[3] Gwinner, J. (1989). A penalty approximation for a unilateral contact problem in non-linear elasticity. Mathematical Methods in the Applied Sciences, 11(4), 447-458.

[4] Gwinner, J. (2022). On a frictional unilateral contact problem in nonlinear elasticity -existence and smoothing procedure. Philos. Trans. Roy. Soc. A, 380, no. 2236, Paper No. 20210356.

S15: Uncertainty quantification

Organizer(s): **Rosic, Bojana** *(U Twente)*
Litvinenko, Alexander *(RWTH Aachen)*

S15-01: Uncertainty quantification

Date: May 30, 2023 13:30-16:10
Room: POT/13

Metropolis-adjusted interacting particle sampling

Sprungk, Bjoern *(TU Bergakademie Freiberg, Germany)* 13:30
Weissmann, Simon *(Universität Mannheim, Germany)*
Zech, Jakob *(Universität Heidelberg, Germany)*

In recent years, several interacting particle samplers have been proposed in order to sample approximately from a complicated target distributions such as posterior measures occuring in Bayesian inverse problems.These interacting particle samplers use an ensemble of interacting particles moving in the product state space according to coupled stochastic differential equations. In practice, we have to apply numerical time stepping to simulate these systems, such as the Euler-Maruyama scheme. However, the time discretization affects the invariance of the particle system with respect to the target distribution and, thus, introduces a bias. In order to correct for this we study the application of a Metropolisation step similar to the Metropolis-adjusted Langevin algorithm. We discuss ensemble- and particle-wise Metropolization and state the basic convergence of the resulting ensemble Markov chain to the product target distribution. We show the benefits of this correction in numerical examples for common interacting particle samplers such as the affine invariant interacting Langevin dynamics (ALDI), consensus-based sampling, and stochastic Stein variational gradient descent.

Data sparse multilevel covariance estimation in optimal complexity

Dölz, Jürgen *(University of Bonn, Germany)* 14:10

We consider the H^2-formatted compression and computational estimation of covariance functions on a compact set in R^d. The classical sample covariance or Monte Carlo estimator is prohibitively expensive for many practically relevant problems, where often approximation spaces with many degrees of freedom and many samples for the estimator are needed. In this article, we propose and analyze a data sparse multilevel sample covariance estimator, i.e., a multilevel Monte Carlo estimator. For this purpose, we generalize the notion of asymptotically smooth kernel functions to a Gevrey type class of kernels for which we derive new variable-order H^2-approximation rates. These variable-order H^2-approximations can be considered as a variant of hp-approximations. Our multilevel sample covariance estimator then uses an approximate multilevel hierarchy of variable-order H^2-approximations to compress the sample covariances on each level. The non-nestedness of the different levels makes the reduction to the final estimator nontrivial and we present a suitable algorithm which can handle this task in linear complexity. This allows for a data sparse multilevel estimator of Gevrey

covariance kernel functions in the best possible complexity for Monte Carlo type multilevel estimators, which is quadratic. Numerical examples which estimate covariance matrices with tens of billions of entries are presented.

Bayesian Inversion Using Generative Machine Learning Models for EIT

Ernst, Oliver *(TU Chemnitz, Germany)*
Gerth, Daniel *(TU Chemnitz, Germany)* 14:30

Electrical Impedand Tomography (EIT) is an imaging modality based on reconstructing a distribution of electrical conductivity or capacitance from the observation of voltages at electrodes on an object's boundary excitation currents injected at pairs of boundary electrodes. The diffusive nature of the physical process results in a notoriously ill-posed inverse problem. We consider a Bayesian formulation based on variational inference using machine learning techniques of (conditional) variational autoencoders and (conditionel) generative adversarial networks. Initial resulta on phantom benchmarks indicate the potential of imptoved reconstructions over standard approaches.

Bayesian sparse self-organized maps

Rosic, Bojana *(University of Twente, Netherlands, The)*
van de Weg, Bram *(University of Twente, Netherlands, The)* 14:50

The discretization of parametric partial or ordinary differential equations describing complex physical phenomena leads to high-dimensional problems, the solution of which requires a massive computational effort. To address this challenge, the development of low-cost surrogates in a data driven manner is the main focus of this talk. To incorporate prior knowledge as well as measurement uncertainties in the traditional neural networks, an efficient sparse Bayesian training algorithm is introduced. By fine tuning specially designed priors the proposed scheme automatically determines relevant neural connections and adapts accordingly in contrast to the classical gradient-like solution. Due to its flexibility, the new scheme is less prone to overfitting, and hence can be used to approximate both forward and inverse maps by use of a smaller data set. The optimal choice of the measurement data then can be easily achieved by maximizing the information gain. In this talk the new type of learning will be showcased on a high-dimensional stochastic partial differential equation describing the nonlinear mechanics problem, as well as on the Lorenz type of time dependent problem.

On definitions of modes and MAP estimators

Klebanov, Ilja *(Free University of Berlin, Germany)* 15:10

While modes of a probability measure (and thereby maximum a posteriori estimators in the context of Bayesian posteriors) with a continuous Lebesgue density are easy to define, their definition in arbitrary metric spaces, in particular infinite-dimensional Banach and Hilbert spaces, is far from unambiguous. Several definitions, based on "small ball probabilities", have been suggested in the recent years – strong, weak and generalized modes – and many other meaningful alternatives are possible. In fact, even for (discontinuous) Lebesgue densities in

one dimension, the connections between these notions are open problems and there are a lot of interesting questions, which I will present using several novel and insightful examples.

Practical Uncertainty Quantification in Non-Linear Finite Element Simulations using Gaussian Error Propagation

Hartmann, Stefan *(TU Clausthal, Germany)*
Dileep, Pranav Kumar *(TU Clausthal, Germany)*
Müller-Lohse, Lutz *(TU Clausthal, Germany)*
Tröger, Jendrik-Alexander *(TU Clausthal, Germany)*

15:30

Non-linear finite element simulations are based on both uncertain material parameters as well as imperfect boundary conditions. Modern concepts of uncertainty quantification require the modification of finite element programs. Thus, a different – and more practical – approach is followed, where a commercial finite element program is chosen. Gaussian error propagation can be interpreted as the norm of the Gateaux-derivative in a Taylor-series, where the direction is defined by the uncertainty of the influencing parameters. On the basis of forming processes of sandwich sheets made of steel surface layers and glass-fiber reinforced PA6 kernel layers, the concept of Gaussian error propagation is investigated. Thus, a careful investigation of the parameter identification for chosen steel and the fiber-reinforced polymer has to be addressed to estimate the uncertainty of the parameters. The validation example of a deep drawing process is carefully studied using digital image correlation data, where the surface strain determination is performed using triangulation and radial basis function approaches. Experience states that the geometric influences significantly affect the uncertainties of the simulation model. Thus, their uncertainty is estimated as well. Then, the analysis offers the possibility to study the individual contributions in the uncertainty analysis. All numerical results are represented here by error considerations and uncertainty assessments.

S15-02: Uncertainty quantification

Date: May 31, 2023 08:30-09:30
Room: POT/13

On Uncertainty Quantification of Eigenpairs with Higher Multiplicity

Dölz, Jürgen *(University of Bonn, Germany)* 08:30
Ebert, David *(University of Bonn, Germany)*

We consider generalized variational eigenvalue problems with random perturbations in the bilinear forms. This setting is motivated by Galerkin discretizations of the Helmholtz equation or Maxwell's equations with random material laws, for example. The considered eigenpairs can be of higher but finite multiplicity. We investigate stochastic quantities of interest of the eigenspaces and discuss why, for multiplicity greater than 1, only the stochastic properties of the eigenspaces are meaningful, but not of individual eigenpairs. To that end, we characterize the Fréchet derivatives of the eigenpairs with respect to the perturbation and provide a new linear characterization for eigenpairs of higher multiplicity. Based on the Fréchet derivatives of the eigenpair we discuss a meaningful sampling strategy for multiple eigenvalues and develop an uncertainty quantification perturbation approach. In the latter, the arising tensor equations for the covariance can be efficiently solved by a low-rank method, although alternate approaches such as sparse grids are also feasible. Finally, we discuss performance gains compared to sampling based methods.

Efficient solution of the covariance eigenvalue problem for stationary random fields

Zhang, Chao *(TU Chemnitz, Germany)* 08:50
Ernst, Oliver *(TU Chemnitz, Germany)*

The Karhunen-Loève expansion has been a common approach in approximating random fields, but its application to large-scale problems is still challenging due to the difficulty in solving the underlying Fredholm integral eigenvalue problem. In this work, we present a numerical solution approach that efficiently approximates the dominant eigenpairs of the covariance operator of stationary random fields. Our method combines advanced quadrature from the boundary element method with fast matrix-vector multiplication based on hierarchical matrix approximation as well as Krylov-based methods for approximating eigenpairs. Specifically, we employ the Sauter-Schwab quadrature scheme for accurate evaluation of the double integrals from discretizing the kernel operator with the Galerkin method. This scheme mitigates the singularity of the integrals in the case of coincident, common-edge, and common-vertex elements. We then use the hierarchical matrix to approximate the Galerkin system matrix, allowing us to efficiently store the dense matrix and perform matrix-vector multiplication. Finally, we solve the resulting eigenvalue problem using the thick-restart Lanczos method. Numerical results demonstrate the effectiveness of the combined use of these techniques in approximating random fields.

On analytic and Gevrey class regularity for parametric elliptic eigenvalue problems

Chernov, Alexey *(Universität Oldenburg, Germany)*
Le, Tung *(Universität Oldenburg, Germany)*

09:10

We investigate a class of parametric elliptic eigenvalue problems where the coefficients (and hence the solution) may depend on a parameter y. Understanding the regularity of the solution as a function of y is important for construction of efficient numerical approximation schemes. Several approaches are available in the existing literature, e.g. the complex-analytic argument by Andreev and Schwab (2012) and the real-variable argument by Gilbert et al. (2019+). The latter proof strategy is more explicit, but, due to the nonlinear nature of the problem, leads to slightly suboptimal results. In this talk we close this gap and (as a by-product) extend the analysis to the more general class of coefficients.

S15-03: Uncertainty quantification

Date: June 1, 2023 08:30-10:30
Room: POT/13

Stochastic Galerkin method and port-Hamiltonian form for second-order differential equations

Pulch, Roland *(Universität Greifswald, Germany)* 08:30

We consider linear dynamical systems consisting of second-order ordinary differential equations (ODEs), which include an input and a quantity of interest as output. Physical parameters are modelled as random variables to perform an uncertainty quantification (UQ). A polynomial approximation is arranged for the random-dependent state variables as well as the quantity of interest, where orthogonal basis polynomials are applied. A stochastic Galerkin method yields a larger deterministic system of second-order ODEs, which inherits the structure of the original system. Both the original system and the stochastic Galerkin system can be formulated as a port-Hamiltonian system of first order. Each port-Hamiltonian system implies a Hamiltonian function, which describes an internal energy. We examine the properties of the Hamiltonian function in the case of the stochastic Galerkin method. It turns out that the Hamiltonian function of the stochastic Galerkin system represents the expected value of an approximation for the Hamiltonian function of the original random-dependent system. Finally, we present numerical results using a second-order system of ODEs, which models a mass-spring-damper configuration in mechanics.

A Sampling-free Statistical Finite Element Method in Computational Mechanics

Narouie, Vahab *(Institut für rechnergestützte Modellierung im Bauingenieurwesen, TU Braunschweig, Germany)*
Wessels, Henning *(Institut für rechnergestützte Modellierung im Bauingenieurwesen, TU Braunschweig, Germany)*
Römer, Ulrich *(Institut für Dynamik und Schwingungen, TU Braunschweig, Germany)* 08:50

We address the combination of sensor data and computational predictions in mechanics with the statistical finite element method (statFEM), which has been recently introduced as a physics-constrained data regression technique [1]. Here, we adopt a mechanics perspective, where the material coefficients exhibit uncertainties, and the model predicts the displacement field. Following the statFEM paradigm, we first conduct a probabilistic finite element analysis with a stochastic material parameter and the Polynomial Chaos method [2]. We, thereby, explicitly account for model error with a Gaussian process model, where the hyperparameters are updated together with the displacement field. Contrary to Bayesian parameter updating [3], in statFEM, the stochastic material coefficients remain unchanged. Therefore, we assume a stochastic calibration step has already been carried out, and we focus on online prediction based on sensor and simulation data. In particular, the stochastic material coefficient is used within a mechanical model to compute a physically motivated prior for updating and predicting the displacements. In this contribution, we represented the stochastic

displacement field, the model-reality mismatch, and the error with three independent random fields in a suitable Polynomial Chaos basis. The immediate challenge is to combine the mentioned Chaos bases into one unified basis, which allows us to represent an extended Polynomial Chaos-based statistical generating model. We then use the Kalman filter to update the PC coefficients of the stochastic displacement field, building on ideas presented in [3]. Given these coefficients, we can efficiently compute the mean value and covariance of posterior displacement without sampling. We choose a two-dimensional Timoshenko-Goodier cantilever beam with a linear elastic material model and uncertain Young's modulus as a numerical example. Young's modulus is described with the Karhunen-Loève expansion as a lognormal random field. The Polynomial Chaos-based statFEM approach features several advantages; in particular, the data update can be carried out online. Hence, the method is ideal for digital twinning with uncertainty quantification.

References:

[1] M. Girolami, E. Febrianto, G. Yin, F. Cirak. The statistical finite element method (statFEM) for coherent synthesis of observation data and model predictions, Computer Methods in Applied Mechanics and Engineering 375, 113533, 2021.

[2] R. G. Ghanem, P. D. Spanos Stochastic finite elements: a spectral approach, Courier Corporation, 2003.

[3] B. V. Rosic, A. Litvinenko, O. Pajonk, and H. G. Matthies. Sampling-free linear Bayesian update of polynomial chaos representations, Journal of Computational Physics 231(17), 5761-5787, 2012.2

Data-driven domain decomposition describing nonlinear mechanical response of battery cells

Gödde, Timm *(University of Twente, Netherlands, The)* 09:10
Rosic, Bojana *(University of Twente, Netherlands, The)*

Battery cells are subjected to different load case scenarios depending on their use. In automotive applications they undergo large deformations affected by variations in material properties, geometrical features and boundary conditions. To study battery mechanical behavior under different loading conditions, one has to run computationally intensive finite element models that include multiscale analysis.

In this talk a mesh-free method based on the domain decomposition for solving nonlinear mechanical response of a battery cell including uncertainties will be presented. The main idea is to substitute the finite element method by a corresponding surrogate model such as a neural network or a physics informed neural network. We study the combination of domain decomposition methods with data-driven surrogate modelling. The challenging issue in this approach is the definition of the interface condition. In this talk two different strategies will be used: one based on the classical approach, and another in which the decomposition method is substituted by a data-driven learning of the interface. Both approaches will be showcased on a simple example of a homogeneous battery cell with varying material properties.

Estimation of the probability of failure bounds for metal foam structures

Kaupp, Jonas *(Karlsruhe Institute of Technology, Germany)*
Proppe, Carsten *(Karlsruhe Institute of Technology, Germany)*
09:30

Manufacturing process and material imperfections cause a heterogeneous microstructure in metal foams and consequently uncertainties leading to a structural problem for which a failure probability can be computed. In case that the required representative volume element of the microstructure is very large and scale separation does not hold, a statistical volume element leads to apparent material parameters (AMPs) instead of effective parameters. These have to be described by random fields. As a result of applying kinematically uniform and stress-uniform boundary conditions to a sample, upper and lower bounds for the AMPs are acquired. A sufficient number of samples lead to a random field representation for the upper and lower bounds of the AMPs. After discretization, they can be expressed by probability boxes (p-boxes) if no homogenization scheme is used. This contribution aims at propagating the resulting p-boxes through an exemplary system leading to an estimation of the probability of failure bounds with the moving particles algorithm.

Enhancing Structural Design Procedures by Evaluating Polymorphic Uncertain Quantities using Information Reduction Measures

Böttcher, Maria *(Institute for Structural Analysis, TU Dresden, Germany)*
Graf, Wolfgang *(Institute for Structural Analysis, TU Dresden, Germany)*
Kaliske, Michael *(Institute for Structural Analysis, TU Dresden, Germany)*
09:50

The numerical design procedure of a structure is a complex challenge. The structure not only needs to be able to carry the predicted loads, but also has to fulfill a variety of additional criteria. These include, e.g., requirements for sustainability, economics, reliability, resilience or aesthetics, and are based on the specific task at hand.

In order to optimize a structure, the numerical simulation needs to depict the reality as accurately as possible. Therefore, the consideration of the design parameters' uncertainties is crucial, since deviations from the actual structure to the initial design are inevitable. The influences of these data uncertainties on the uncertainty of the structural response is investigated by a robustness evaluation. Especially for nonlinear systems, a small variation of the design parameters can lead to a large change in the structural response. An adequate modeling of the design parameters' uncertainties is fundamental, taking into consideration both aleatoric and epistemic uncertainty in combined form as polymorphic uncertain variables. Uncertainty analyses yield uncertain output quantities, i.e. uncertain structural responses, which represent the magnitude of the variation resulting from uncertain input. To include this information in the design optimization, these uncertain output quantities are post-processed in order to gain relevant insights regarding the robustness as well as the performance. For this purpose, information reduction measures (IRMs), classified into representative measures and uncertainty quantifying measures, are applied. Various measures exist, but clear recommendations or explanations why certain measures are selected in examples are scarce despite the fact that different characteristics of the uncertain output quantities are accounted for with different measures.

The focus of this contribution lies on investigating and comparing commonly applied IRMs to help users navigate the choice of appropriate measures for their task. This includes insights into, e.g., sensitivity towards skewness of random variables' distributions and implementation and computational effort. An example of a simplified structural design process is used to highlight similarities and differences. The aim is to provide a guide as to which ïnformationï̈s reflected by each of the investigated IRMs.

Furthermore, the results of nested stochastic and fuzzy analyses for structural designs with polymorphic uncertain variables, are discussed. This includes the investigation of how the different origins of input parameter uncertainty - aleatoric and epistemic - contribute to resulting value of each of the IRMs. Additionally, improvements regarding the interpretability of these values are presented and illustrated by examples.

S15-04: Uncertainty quantification

Date: June 2, 2023 11:00-13:00
Room: POT/13

The MISC method for uncertainty quantification in engineering problems

Piazzola, Chiara *(Technische Universität München, Germany)*
Tamellini, Lorenzo *(Consiglio Nazionale delle Ricerche, Italy)*
11:00

In this talk we discuss recent advances on the use of Multi-Index Stochastic Collocation (MISC) for Uncertainty Quantification of PDEs with uncertain parameters, and show its application to engineering problems. MISC is a multi-fidelity method that extends the Multi-Level Monte Carlo approach, replacing the Monte Carlo sampling at each level with a sparse-grid sampling, and therefore can also be used to compute a multi-fidelity metamodel for the PDE, i.e., a multi-fidelity approximation of the function mapping the values of the uncertain parameters to the corresponding solution of the PDE (also known as response surface). This approximation is provably convergent under suitable regularity assumptions of such mapping and if the different fidelities considered are obtained by a suitable sequence of mesh refinement to be used for the PDE solver.

References:

C. Piazzola, L. Tamellini, R. Pellegrini, R. Broglia, A. Serani, and M. Diez. Comparing Multi-Index Stochastic Collocation and Multi-Fidelity Stochastic Radial Basis Functions for Forward Uncertainty Quantification of Ship Resistance. Engineering with Computers, 2022.

J. Beck, L. Tamellini, and R. Tempone. IGA-based Multi-Index Stochastic Collocation for random PDEs on arbitrary domains. Computer Methods in Applied Mechanics and Engineering, 2019

Uncertainty quantification in the coastal aquifers using Multi Level Monte Carlo

Litvinenko, Alexander *(RWTH Aachen, Germany)*
Logashenko, Dmitry *(KAUST, Saudi Arabia)*
Tempone, Raul *(RWTH Aachen, Germany; KAUST, Saudi Arabia)*
Vasilyeva, Ekaterina *(Goethe-Universität Frankfurt am Main, Germany)*
Wittum, Gabriel *(KAUST, Saudi Arabia)*
11:40

We consider a class of density-driven flow problems. Particularly, we are interested in the problem of the salinisation of coastal aquifers. As a test case, we consider the Henry saltwater intrusion problem with uncertain porosity, permeability, and recharge parameters. The reason for the presence of uncertainties is the lack of knowledge, inaccurate measurements and inability to measure parameters at each spatial or time location. This problem is nonlinear and time-dependent. The solution is the salt mass fraction, which is also uncertain and changes in time. Uncertainties in porosity, permeability, recharge, and mass fraction are modelled by random fields. The goal of this work is to investigate the applicability of the well-known Multi Level Monte Carlo (MLMC) method for such types of problems. MLMC is able to reduce the total computational and storage costs. MLMC runs multiple scenarios on different spatial and time meshes, and then estimates the mean value of the mass fraction. The

parallelization is done in both - the physical space and the stochastic space. To solve every deterministic scenario, we run the parallel multigrid solver ug4 in a black-box fashion. As a reference solution we used the QMC solution.

Data-driven model order reduction in subset simulations

Thaler, Denny *(Institute of General Mechanics, RWTH Aachen University, 52062 Aachen, Germany)*
Shields, Michael D. *(Department of Civil and Systems Engineering, Johns Hopkins University, 3400 N. Charles St., Baltimore, MD 21218, USA)*
Markert, Bernd *(Institute of General Mechanics, RWTH Aachen University, 52062 Aachen, Germany)*
Bamer, Franz *(Institute of General Mechanics, RWTH Aachen University, 52062 Aachen, Germany)*
12:00

The crude Monte Carlo method is computationally expensive. Hence, incorporating model order reduction methods enables reliability analysis for high-dimensional problems is necessary [1]. However, this strategy may result in an inaccurate estimation of the probability of failure for rare events for two main reasons. First, the data-driven model order reduction, i.e., proper orthogonal decomposition, requires samples from the region a priori. Thus, we propose to update the proper orthogonal modes using extreme events. Second, the crude Monte Carlo simulation requires many samples to estimate low failure probabilities reliably. To this end, subset simulation found wide application in reliability analysis to reduce computational effort [2]. Following this strategy, the proposed samples gradually move toward the failure region. Thus, incorporating updates of the modes is particularly promising in evaluating samples from the current subset region. This contribution shows the computational efficiency of proper orthogonal decomposition within subset simulations. We then propose to leverage the estimation of the probability of failure by updating the modes within each subset.

Literature:

[1] F. Bamer, B. Markert, Mech. Based Des. Struct. Mach. 45 (2017) 313-330.
[2] S.K. Au, J.L. Beck, Probab. Eng. Mech. 16 (2001) 263-277.

On probabilistic entropies application in uniaxial deformation of hyper-elastic materials

Kamiński, Marcin *(Lodz University of Technology, Department of Structural Mechanics, Poland)*
12:20

The main aim is to demonstrate an application of probabilistic entropy and probabilistic relative entropy in engineering analyses of hyper-elastic materials. Various constitutive models of such materials include the neo-Hookean, Mooney-Rivlin, Yeoh, Gent, Arruda-Boyce, and also the Extended Tube approaches rewritten in the context of uncertainty analysis. These constitutive relations are tested on the example of the uniaxial tension of incompressible material documented by Treloar. A deformation of a rubber specimen is treated as a Gaussian random variable having a priori given expectation and standard deviations varying within the given experimental bounds. Probabilistic analysis is provided here in three alternative ways—via the traditional Monte-Carlo technique, using a semi-analytical probabilistic approach as well as

with the use of higher order stochastic perturbation technique. This analysis includes computational determination of the first four basic probabilistic characteristics, i.e. expectation, coefficient of variation, skewness, and kurtosis, and is provided to verify the resulting probabilistic distribution of the induced stress and its entropy. Shannon entropy is calculated here to give an alternative uncertainty propagation measure to the second-order moment, whereas Bhattacharyya distance is employed to formulate some reliability criterion in hyperelasticity.

S15-05: Uncertainty quantification

Date: June 2, 2023 16:00-18:00
Room: POT/13

Applied Bayesian Structural Health Monitoring: inclinometer data anomaly detection and forecasting

Green, David K. E. *(DYWIDAG, United Kingdom)* 16:00
Jaspan, Adam *(DYWIDAG, United Kingdom)*

Inclinometers can be used to measure deformations within earthwork slopes. This paper demonstrates novel Bayesian anomaly detection and forecasting techniques applied to real world inclinometer data. Specifically, we use data collected from across the entire UK rail network.

Practitioners have, effectively, two goals when processing monitoring data. The first is to identify any anomalous or dangerous movements. The second is to predict potential future adverse scenarios by forecasting. We demonstrate novel anomaly detection and forecasting for inclinometer data using Bayesian techniques.

Although inclinometers are a standard tool of geotechnical analysis, risk analysis and decision-making using anomalies and forecasts from inclinometer data requires significant and subjective 'engineering judgement'. This is because the observational data is derived from complex physical phenomena. The inclinometer time series data contains complex spatio-temporal correlations which makes the data difficult to work with from a statistical perspective. Additionally, the practical demands of data collection from remote sites over several years tends to introduce systematic errors into the data.

We demonstrate both anomaly detection and forecasting on complex inclinometer data using Uncertainty Quantification techniques. By quantifying the appropriate uncertainties, the impact of subjective human engineering judgements can be rigorously assessed. This is an enabler for enhanced decision making and risk analysis frameworks.

We show that a latent model autocorrelated Markov model for inclinometer data can be derived from site observations and instrument measurements. This model can be used as the transition model for a nonlinear Bayesian filter. This allows for the prediction of future observations. This learnt latent model also allows for the detection of anomalies: future observations that are far from model predictions can be considered to have 'high surprisal', that is they have a high information content relative to the model encoding represented by the learnt latent model.

We additionally demonstrate that systematic errors from the measurements must be removed to form an adequate latent model. This removal of systematic errors requires knowledge of the slope geometry, data that can not be inferred from the inclinometer data itself. This raises interesting questions regarding how much can be achieved with purely 'model-free' techniques.

We successfully apply the forecasting and anomaly detection techniques to a large real world data set in a computationally efficient manner. Although this paper studies inclinometers in particular, the techniques are broadly applicable to all areas of engineering Uncertainty Quantification and Structural Health Monitoring.

Stochastic buckling loads of thin-walled structures combining linear and nonlinear analysis

Fina, Marc *(Institute for Structural Analysis, Karlsruhe Institute of Technology, Germany)*
Wagner, Werner *(Institute for Structural Analysis, Karlsruhe Institute of Technology, Germany)*
Freitag, Steffen *(Institute for Structural Analysis, Karlsruhe Institute of Technology, Germany)*
Valdebenito, Marcos A. *(Chair for Reliability Engineering, TU Dortmund University, Dortmund, Germany)*
Faes, Matthias G.R. *(Chair for Reliability Engineering, TU Dortmund University, Dortmund, Germany)*
Broggi, Matteo *(Institute for Risk and Reliability, Leibniz University Hannover, Germany)*
Beer, Michael *(Institute for Risk and Reliability, Leibniz University Hannover, Germany)*
16:20

Buckling is the most significant failure mode for thin-walled structures. Even small variations of geometrical and material imperfections have a major influence on the buckling behavior. Therefore, it is essential to consider uncertainties. The calculation of stochastic buckling loads, e.g. with the Monte-Carlo simulation, can be computationally expensive. When a linear pre-buckling behavior is present, the buckling load can be calculated with a linear buckling analysis. The results of linear analysis can strongly differ from the true buckling load in case of a non-linear pre-buckling behavior. Then a nonlinear buckling analysis is required, where a completely geometrically nonlinear path following analysis with the application of an iteration procedure has to be performed. This can be computationally very expensive using the Monte Carlo simulation. In this paper the second-order statistics (mean and standard deviation) of buckling loads are estimated by control variates. Thus, the existing correlations between the solutions of a linear and nonlinear buckling analysis are exploited. The idea is to run the more expensive analysis (nonlinear buckling analysis) a few times only, while to run the cheaper linear buckling analysis a considerable number of times. The approach is presented on different thin and slender structures like beams and shells, where the imperfections are characterized by means of probabilistic models.

Non-intrusive operator inference for a soft robot segment

Berghuis, Minke Wilhelmina *(University of Twente, Netherlands, The)*
Stanić, Andjelka *(University of Twente, Netherlands, The)*
Rosic, Bojana *(University of Twente, Netherlands, The)*
16:40

Physics based modeling of nonlinear continuous structures often requires computationally expensive numerical models. These predictive models are build from observations on the material behaviour and first principles. While offering freedom in the simulated parametric structure designs, materials and loading conditions, the spatial discretization and nonlinear description of these models yield high dimensional systems that are expensive to evaluate. However, applications in design optimization and control depend on fast model evaluations. Reducing the computational expense of these predictive models is thus desirable.

Model order reduction (MOR) strives to preserve the structure and simulation freedom of the physics based full order models (FOMs) while significantly decreasing the computational burden. The reduced order model (ROM) response should approximate the response of the FOM according to specific well-defined criteria. Efficient MOR techniques exist based on projection of the FOM states and operators onto a reduced basis (modal reduction, moment matching, balanced truncation). However, these intrusive methods all require the availability of the FOM operator (white box model). These operators may not be available explicitly, for example in commercial computational software, which therefore prevents the intrusive projection step.

This work focuses on non-intrusive MOR by assuming a physics based ROM model structure (grey box model). In particular, the FOM adopted in this work is a nonlinear finite element model (FEM) of a soft continuous robot arm. *Soft robots* are highly compliant structures, on account of their soft material and/or geometry. Soft continuous arms enable types of manipulation different from their rigid body counterparts, such as whole-arm grasping and compliant pick-and-placing. Their ROM operators are inferred using energy observations from the expensive black box FOM.

Parameter identification in dynamic crack propagation modelled by ED-FEM

Stanić, Andjelka *(University of Twente, Faculty of Engineering Technology, The Netherlands)* 17:00
Nikolić, Mijo *(University of Split, Faculty of Civil Engineering, Architecture and Geodesy, Croatia)*
Friedman, Noemi *(Institute for Computer Science and Control (SZTAKI), Hungary)*
G. Matthies, Hermann *(Technische Universität Braunschweig, Institute of Scientific Computing, Germany)*

The subject of our research work is the identification of material parameters in a numerical model, that enables simulation of crack propagation in a structural element subjected to dynamic loads. In order to describe a crack formation and opening in quasi brittle 2d solid we use the embedded strong discontinuity method (ED-FEM). It provides mesh-independent solution since the fracture dissipation energy is associated with the discontinuity and does not depend on the finite element size. In this work we use two different finite element models with embedded strong discontinuity: the lattice element and the quadrilateral Q6 element. Since the lattice model is a discrete model of continuum, we calibrate the stiffness matrix of a lattice element first. Then we use the stochastic Bayesian inverse method to estimate the input material parameters, that cannot be measured directly - such as the fracture energy which dissipates when cracks propagate through the model domain. As the representative example of fracture dynamics, we consider the Kalthoff's test on a high-strength steel plate.

Time-separated stochastic mechanics for the simulation of locally fluctuating viscoelastic materials with application to composites

Geisler, Hendrik *(Leibniz University Hannover, Germany; IRTG 2657: Computational Mechanics Techniques in High Dimensions; Université Paris-Saclay, CentraleSupélec, ENS Paris-Saclay, CNRS, LMPS - Laboratoire de Mécanique Paris-Saclay, Gif-sur-Yvette, France)*
Junker, Philipp *(Leibniz University Hannover, Germany; IRTG 2657: Computational Mechanics Techniques in High Dimensions)*

17:20

The realistic modelling of structures with inherent uncertainties, e.g. specifically uncertainties in the material properties, is fundamental for a precise assessment of its reliability. However, inelastic material behavior and local material fluctuations render simulations typically computationally expensive. This severly hinders the widespread use of stochastic information in engineering computations. The time-separated stochastic mechanics is a novel technique developed for the precise yet computationally efficient estimation of the stochastic characteristics of inelastic structures with random material properties. It is based on a separation of both the system equation, i.e. the balance of linear momentum, and the evolution equation for a visco-elastic material into stochastic and deterministic terms. Then, only a low number of deterministic FEM simulations and several fast matrix calculations are needed to approximate the stochastic behavior. In this talk, we present how the method can be adapted for local material fluctuations by combination with the Karhunen-Loéve expansion. Further, an application for the computational homogenization of composite materials is given. In doing so, the number of FEM simulations required can be drastically reduced compared to the classic Monte Carlo method.

Modelling and estimation of the reliability of electrical components for autonomous driving

Kimmerle, Sven-Joachim *(TH Rosenheim, Germany; Physical Software Solutions GmbH, Ottobrunn, Germany)*

17:40

From automated to autonomous cars, a higher and higher reliability of the electrical components is required, while on the other hand the number of electric components is continuously increasing in modern cars. Therefore for these components the estimation of a TTF (time-to-failure) and a failure rate, a so-called FIT (failure-in-time) rate, and the quantification of the corresponding uncertainties is crucial. The verification of required FIT rates of less than 1 FIT i.e. 1 failure in 1 billion hours of life time are a challenge. [1]
These risk measures have to be determined before and within the development process of future automated/autonomous cars. However, tests in real time take too long (the lifetime of a car is calculated here with 15 years) and are too expensive. Moreover the uncertainty quantification of networks of components as in vehicle electric systems has to be considered as well.

There are the following options:

1. Experimental tests accelerated by overstresses, requiring accepted laws (e.g. the Arrhenius law) for relating different stress levels to each other

2. Estimation of failure rates by catalogues or standards (as MIL-HDBK 217F, SN 29500-1, and most recently the FIDES guide [2])
3. Evaluation of data, so-called field data, from past records of car manufacturers, if available and provided
4. Simulations of the interplay of failures in complex systems

Following an overview the talk will focus on approach 1. and the combination of overstresses varying in time [3]. Mathematically, the latter means a switching between different probability distributions in time. The results call into question whether the consideration of temperature collectives is applicable here, since the temporal order of the stresses is essential.
This is joint work in parts with Prof. Dr.-Ing. H.-D. Liess and Prof. Dr. R. Avenhaus (both UniBw München at Neubiberg). The research has been motivated by several industrial projects.

References:

[1] Technischer Leitfaden: Ausfallraten für Bordnetz-Komponenten - Erwartungswerte und Bedingungen (1st ed.). ZVEI e.V., Frankfurt a. M. & Bayern Innovativ, Cluster Automotive, Nürnberg, 2021.
[2] FIDES Guide 2009 Edition A, Reliability Methodology for Electronical Systems (revised version). Institut pour la Maîtrise des Risques, Gentilly, France, 2010.
[3] Kimmerle, Sven-Joachim; Dvorsky, Karl; Ließ, Hans-Dieter; Avenhaus, Rudolf: Time to Failure under Varying Thermal Stresses. Preprint-Server OPUS der TH Rosenheim, Nr. 1912 (2022), urn:nbn:de:bvb:861-opus4-19126. Submitted.

S16: Optimisation

Organizer(s): **Schwartz, Alexandra** *(TU Dresden)*
Joormann, Imke *(TU Braunschweig)*

S16-01: Optimisation

Date: May 30, 2023 13:30-16:10
Room: HSZ/105

Mixed-integer NMPC for real-time supervisory control of buildings' energy management

Bitner, Dimitri *(Institute of Engineering Design, Mechatronics and Electromobility (IKME), Hannover University of Applied Sciences and Arts, Germany)*
Burda, Artyom *(Institute of Engineering Design, Mechatronics and Electromobility (IKME), Hannover University of Applied Sciences and Arts, Germany)*
Grotjahn, Martin *(Institute of Engineering Design, Mechatronics and Electromobility (IKME), Hannover University of Applied Sciences and Arts, Germany)*
Kirches, Christian *(Institute for Mathematical Optimization, Technische Universität Carolo-Wilhelmina zu Braunschweig, Germany)*
Schild, Axel *(IAV GmbH, Germany)*
Luck, Bennet *(IAV GmbH, Germany)*

13:30

Over the last years a boost in building energy supply and distribution systems' complexity is particularly evident. The number of energy generators, storages, flows, and the variety of their combinations are constantly rising. Thus, the required supervisory control becomes particularly challenging - especially under the conflicting goals of comfort maximization as well as cost and emission minimization. The last one is of a significant importance due to global climate protection goals and the associated transformation to sustainable energy production. A promising candidate for an intelligent real-time supervisory control system is a model predictive control (MPC) strategy. Of particular interest is nonlinear MPC (NMPC), which can be directly applied to nonlinear multidimensional systems, as they occur in the building sector. We present an even more advanced case of NMPC, mixed-integer NMPC (MI-NMPC), in order to consider integer controls and restrictions of typical building technology components without considerable problem reformulations. The strategy utilizes a decomposition approach, where an approximation of the optimal solution is determined by combination of sophisticated and rapid convexification and rounding procedures to achieve real time capability. Switch-Cost Aware Rounding (SCARP) allows us to directly tackle the switching behavior of the building components along with minimum admissible operating time constraints. The capacity of the developed approach is proven by a practical application to two real world scenarios: a single-family house with a combined heat and power plant and its extension to a multi-family house with 18 residential units. We briefly summarize the results of a simulation study for the energy system of the single-family house. The real-time performance and the resulting quality of the solution have been proved by their high correspondence to the globally optimal solution calculated by the computationally intensive Dynamic Programming

method. An average optimality gap of 2.5% compared to 20% for a conventional heat-led control approach has been achieved while retaining high computational speed and scalability properties. Moreover, we point out the results of the strategy application to the multifamily residential. In this case, we combine physically-based and data-based modelling approaches in order to achieve sufficient prediction quality of the complex energy system behavior. This results in a complex optimization task with multiple degrees of freedom. However, the simulation again proves high quality and real-time capability of the developed control strategy. Apart from that, we present first results of the controller implementation in the building.

Optimal Yaw Control in Wind Farms by Integer Programming

Bestehorn, Felix *(TU Braunschweig, Germany)*
Bürgel, Florian *(TU Braunschweig, Germany)*
Kirches, Christian *(TU Braunschweig, Germany)*
Stiller, Sebastian *(TU Braunschweig, Germany)*
Tillmann, Andreas M. *(TU Braunschweig, Germany)*
13:50

Wind farms are expected to be one of the main sources of electrical power in the future. Within them, the wakes cased by the wind turbines negatively impact the power generation and load of downstream turbines. The strong interactions between individual wind turbines provide opportunities to increase the power output and/or mitigate the adverse effects during wind farm operation, e.g., by axial induction-based or yaw-based control. We propose an integer programming approach to yaw-based control that allows for globally optimal yaw control. The underlying wind farm yaw problem determines an optimal configuration of the yaw angles for all turbines in the wind farm for a given wind scenario (direction and speed), and needs to be resolved periodically in the control context. We establish strong NP-hardness and inapproximability of the wind farm yaw problem; nevertheless, we demonstrate through numerical experiments that our method allows for its efficient solution in practice and, in particular, enables optimal yaw control under real-world requirements on control update periods.

Using Predictions in Online Combinatorial Optimization

Megow, Nicole *(University of Bremen, Germany)*
14:10

Online optimization refers to solving problems where an initially unknown input is revealed incrementally, and irrevocable decisions must be made not knowing future requests. The assumption of not having any prior knowledge about future requests seems overly pessimistic. Given the success of machine-learning methods and data-driven applications, one may expect to have access to predictions about future requests. However, simply trusting them might lead to very poor solutions as these predictions come with no quality guarantee. In this talk we present recent developments in the young line of research that integrates such error-prone predictions into algorithm design to break through worst case barriers. We discuss algorithmic challenges with a focus on online routing and network design and present algorithms with performance guarantees depending on a novel error metric.

A random preconditioned gradient method for least squares optimization problems

Vater, Nadja *(Julius-Maximilians-Universität Würzburg, Germany)*
Borzì, Alfio *(Julius-Maximilians-Universität Würzburg, Germany)* 14:50

A random preconditioned gradient scheme for the solution of nonlinear least squares problems is presented. The random preconditioner is constructed by employing a random subspace embedding developed in the framework of randomized numerical linear algebra technique [1].
In this talk, theoretical and computational aspects of the proposed preconditioning scheme for a gradient method are discussed. In particular, necessary conditions for the convergence of the method are shown. Further, results of numerical experiments with the resulting preconditioned gradient method are presented. These results demonstrate the effectiveness of preconditioning compared to a standard gradient method.

[1] N. Vater and A. Borzì. Preconditioned Gradient Descent for Data Approximation with Shallow Neural Networks. International Conference on Machine Learning, Optimization and Data Science, 2022 (to appear).

ResQPASS: an algorithm for bound constrained least squares problems

Symoens, Bas *(University of Antwerp, Belgium)*
Vanroose, Wim *(University of Antwerp, Belgium)* 15:10

Inverse problems appear everywhere in scientific and industrial applications. They are often solved through some minimization problem of which a regularized least squares problem is a commonly used example (LASSO, elastic net ...). We are particularly interested in solving a bound constrained least squares problem, since they have various applications in for example machine learning, calibration problems and signal processing and they can be formulated relatively easily. Bound constrained means that we wish to minimize $||Ax-b||^2$ subject to the bound constraints $l \leq x \leq u$. To accomplish this, we have combined techniques from Krylov methods with the QPAS optimization algorithm into our ResQPASS (Residual Quadratic Programming Active Set Subspace) method.Krylov methods are a common tool to solve huge scale linear algebra problems, but have recently also proven very useful in solving certain LP problems. However, the techniques used in these LP problems can't be expanded to QP problems, which is why we attempted to create a generalization.ResQPASS has two main parts: an outer loop and an inner loop. In the outer iterations, a residual based subspace is constructed on which the problem is projected. In this subspace we solve the problem using the QPAS algorithm, which makes up our inner iterations.The residuals that are used, are derived from the projected KKT system and have some nice properties. For one, they are orthogonal and in the unconstrained case, they are exactly the residuals used in a classical Krylov subspace. This implies that our method is a generalization of classical Krylov methods. Moreover, the basis converges toward a Krylov basis, which in turn provides us with superlinear convergence from a certain point on. This point of superlinear convergence occurs once the active set of the solution has been found.Finally, via techniques such as warm-starting, limiting inner iterations, QR updates and Cholesky updates, the ResQPASS method has been sped up significantly.

S16-02: Optimisation

Date: May 31, 2023 14:00-16:00
Room: HSZ/105

Knight descent: a parallel stochastic method for non-linear optimization problems.

Angino, Andrea *(UniDistance Suisse, Switzerland)* 14:00
Kopanicakovà, Alena *(UniDistance Suisse, Switzerland)*
Krause, Rolf *(UniDistance Suisse, Switzerland)*
Donatelli, Marco *(UniDistance Suisse, Switzerland)*

In this talk, we propose a novel class of algorithms, called M-knight descent, to solve unconstrained minimization problems. An M-knight descent method employs a standard optimization method M, called the generator, and exploits the information given by stochastically sampled points to generate the search directions. Its name has no romantic origins, but it is rather derived from the geometric shape of the iterative step. The M-knight descent strategy is a suitable option to solve optimization problems for which the generator M is an appropriate choice. Compared to the method M, the M-knight descent guarantees a higher decrease in the objective function per iteration. Moreover, the proposed M-knight descent algorithm can exploit parallelism, thanks to the independence between samples. We demonstrate the convergence properties and the performance of the M-knight descent method using several numerical examples. Furthermore, the efficiency of the methods is illustrated by a comparison with state-of-the-art unconstrained optimization methods.

A Multilevel Low-Rank Newton Method with Super-linear Convergence Rate and its Application to Non-convex Problems

Tsipinakis, Nick *(UniDistance Suisse, Switzerland)* 14:20
Tigkas, Panagiotis *(University of Oxford, UK)*
Parpas, Panos *(Imperial College London, UK)*

Second-order methods can address the shortcomings of first-order methods for the optimization of large-scale machine learning models. However, second-order methods have significantly higher computational costs associated with the computation of second-order information. Subspace methods that are based on randomization have addressed some of these computational costs as they compute search directions in lower dimensions. Even though super-linear convergence rates have been empirically observed, it has not been possible to show that these variants of second-order methods can indeed achieve such fast rates. Yet, it is not clear whether subspace methods can be applied to non-convex cases. We develop a link between multigrid optimization methods and low-rank Newton methods that enables us to prove the super-linear rates of stochastic low-rank Newton methods rigorously. Our method does not require any computations in the original model dimension. We further propose a truncated version of the method that is capable of solving high-dimensional non-

convex problems. Preliminary numerical experiments show that our method has a better escape rate from saddle points compared to accelerated gradient descent and Adam and thus returns lower training errors.

SLEQP: An Open Source Package for Nonlinear Programming

Hansknecht, Christoph *(TU Clausthal, Germany)*
Kirches, Christian *(TU Braunschweig, Germany)*
14:40

We present SLEQP, an open source C-package consisting of an active-set method capable of solving large-scale nonlinear programming problems based on successive linear programming and equality constrained quadratic programming techniques. The method includes a feasibility restoration phase and second-order corrections, achieing robust practical performance. It has also been adapted for the special cases of unconstrained optimization, box-constrained problems, and nonlinear least squares problems and contains interfaces to both Python and MATLAB. To demonstrate the performance of the package, we perform a computational study based on the well-known CUTest suite of nonlinear programming problems.

Sequential optimality conditions for cardinality-constrained optimization problems with algorithmic applications

Kanzow, Christian *(Universität Würzburg, Germany)*
Raharja, Andreas B. *(Universität Würzburg, Germany)*
Schwartz, Alexandra *(TU Dresden, Germany)*
15:00

Following an approach to tackle cardinality-constrained optimization problems using a continuous reformulation, we derive a problem-tailored sequential optimality condition, which is satisfied at every local minimizer without requiring any constraint qualification. We relate this condition to an existing M-type stationary concept by introducing a weak sequential constraint qualification based on a cone-continuity property. Finally, we present two algorithmic applications: We improve existing results for a known regularization method by proving that it generates limit points satisfying the aforementioned optimality conditions even if the subproblems are only solved inexactly. And we show that, under a suitable assumption, any limit point of a standard (safeguarded) multiplier penalty method applied directly to the reformulated problem also satisfies the optimality condition.

Branching Exponents in NLP-Based Synthetic Vascular Trees

Jessen, Etienne *(Technical University of Darmstadt, Germany)*
Steinbach, Marc C. C. *(Leibniz Universität Hannover, Germany)*
Debbaut, Charlotte *(Ghent University, Belgium)*
Schillinger, Dominik *(Technical University of Darmstadt, Germany)*
15:20

Realistic vascular trees can be synthesized by optimization methods based on the physiological assumption that they minimize the total power for maintaining the blood flow. Our recent algorithmic approach generates vascular trees with more than one million vessels efficiently based on a rigorous NLP model of the geometry combined with a Simulated Annealing heuristic for the topology. We solve several NLP variants differing in the precise model assumptions

to study the so-called branching exponents predicted by Murray's law almost 100 years ago based on simplified modeling. In addition to the numerical experiments we will also discuss first theoretical results and give a comparison with the corrosion cast of a human liver.

S16-03: Optimisation

Date: June 1, 2023 08:30-10:30
Room: HSZ/105

Path and Power Optimization of an Electric Airship with Integrated Solarcells

Motyl, Jonas *(Friedrich Alexander Universität, Germany)* 08:30
Pflaum, Christoph *(Friedrich Alexander Universität, Germany)*

Lighter-than-air aircrafts (airships) with integrated solar cells can help to reduce CO_2 emissions of the aviation sector, while reducing the energy costs. To this end, an optimal control of the airship is needed. This includes path optimization and optimal charging and discharging of the battery of the airship. We present an algorithm which performs an optimal control of the airship and takes into account historic wind data and the day-dependent position of the sun. The algorithm is based on different numerical algorithms like A* path search algorithm, a simulated annealing algorithm and a gradient search algorithm. Simulation results show that CO_2 emissions and energy consumption is reduced to less than 5% of a conventional aircraft.

Solar airships are sustainable because they utilize renewable energy from the sun to power their operations, eliminating the need for fossil fuels and reducing greenhouse gas emissions. These airships can travel long distances with minimal impact on the environment, as they do not produce harmful pollutants or contribute to climate change. Additionally, solar airships can be used for a variety of purposes, such as transportation, scientific research, and humanitarian aid, making them a versatile and eco-friendly alternative to traditional modes of transportation. By harnessing the power of the sun, solar airships offer a sustainable solution for the future of transportation and exploration.

Optimal control of the airship is important for estimating and reducing travel time. Without the underlying mathematical algorithms larger batteries are needed and certain destinations cannot be reached.

Optimal Strategies of ISO and Producers on Electricity Markets with Elastic Demand, Production Bounds and Costs

Branda, Martin *(Institute of Information Theory and Automation, Prague, Czech Republic)* 08:50
Allevi, Elisabetta *(Brescia University, Italy)*
Outrata, Jiří *(Institute of Information Theory and Automation, Prague, Czech Republic)*
Pištěk, Miroslav *(Institute of Information Theory and Automation, Prague, Czech Republic)*
Riccardi, Rossana *(Brescia University, Italy)*

Our paper is focused on deriving the optimal strategies of the independent system operator (ISO) and producers on electricity markets with production bounds and costs which are made up mainly of the prices of emission allowances or corresponding derivatives. The ISO works under the demand elasticity and maximizes the social welfare of the market. Each of the producer's problem is a bilevel optimization problem in which the upper level represents the producer's problem of profit maximization, while the lower level optimization problem,

shared by all the producers, is the ISO's problem. This leads to a multi-leader-common-follower model. We formulate the optimality conditions for both problems. We focus on deriving the Clarke subdifferential of the objective function in the bilevel producers problem. This subdifferntial is then used in a bundle method under non-convex settings. Numerical results will be presented.

Application of Parameter Identification for Modelling of Energy Storages in a Smart Energy Management System

Kappertz, Lars *(Universität Bremen, Germany)* 09:10
Dierkes, Eva *(Universität Bremen, Germany)*
Hackenberg, Annika *(Universität Bremen, Germany)*
Solovievskyi, Viacheslav *(Universität Bremen, Germany)*
Büskens, Christof *(Universität Bremen, Germany)*

The growing share of weather-dependent sources of energy like wind or photovoltaic plants is leading to a growing need for demand site management. The lack of control on the side of energy generation is compensated on the demand side by controlling the consuming devices according to the fluctuating amount of generation. The application of databased modelling and numerical optimization methods allows this to be done in a forecast-based, smart energy management system (EMS). Such an EMS can be used, for example, by individual households or enterprises that generate their own renewable energy on-site, to increase their profits by optimizing their self-consumption. A key component of a forecast-based EMS are models that need to provide accurate and robust forecasts of power consumption, generation and storage for all relevant devices. Accurate forecasts are especially important for dynamic systems like energy storages systems, since all forecast errors accumulate over the forecast horizon.

In this work, the application of physics-based parameter identification models is proposed to forecast the behaviour of (thermal) energy storages. With sufficient data, the parameters of physics-based model functions, generally ordinary differential equations (ODEs), can be identified and used to generate appropriate forecasts. The parameter identification problem at the core of the model training process is formulated to find the parameters that minimize the sum of squared errors between model and measurement state values, where the model values are obtained by integrating the model ODE. Here, the direct method of full discretization is used to compute the optimal parameters, thus training the model. The benefits and challenges of developing and using such models are demonstrated based on measurement data from various devices like an electrical battery, a heat pump, or refrigeration systems like freezer or milk cooling tank.

Data-Driven Distributional Robustness with Applications in Material Science and in Energy

Liers, Frauke *(Friedrich-Alexander University Erlangen-Nürnberg, Germany)* 09:30

In many applications, determining optimized solutions that are hedged against uncertainties is mandatory. Classical stochastic optimization approaches, however, may be prone to the disadvantage that the underlying probability distributions are unknown or uncertain themselves. On the other hand, standard robust optimization may lead to conservative results as

it generates solutions that are feasible regardless of how uncertainties manifest themselves within predefined uncertainty sets. Distributional robustness (DRO) lies at the interface of robust and stochastic optimization as it robustly protects against uncertain distributions. DRO currently receives increased attention and is considered as an alternative that can lead to less conservative but still uncertainty-protected solutions. In this talk, we will review some approaches in the area of distributional robustness. We will explain some recent developments that use scenario observations to learn more about the uncertain distributions over time, together with best possible protected solutions. The goal is to incorporate new information when it arrives and to improve our solution without resolving the entire robust counterpart. We also present results for DRO applications in energy and in the design of nanoparticles.

S16-04: Optimisation

Date: June 1, 2023 16:00-19:00
Room: HSZ/105

An experimental validation of simulation results of the thermodynamic topology optimization including plasticity

Kick, Miriam *(Leibniz Universität Hannover, Germany)* 16:00
Junker, Philipp *(Leibniz Universität Hannover, Germany)*

The inclusion of complex real-world material behavior into topology optimization is still challenging. Therefore, we aimed to develop an extension of the thermodynamic topology optimization (TTO) to account for plastic material behavior. The plastic material behavior is computed by a surrogate plasticity model which gives physically correct plastic strains which agree to those of classic elasto-plastic material models. Thus, the simulation results are meaningful and promising. However, it is important to prove whether the method is suitable for real-world applications. In this talk, we present our experimental investigation on thermodynamic topology optimization of elasto-plastic structures using additive manufacturing. Additive manufacturing is the best method to produce topology-optimized structures directly and with sustainable use of materials. Here, a new technology of additive manufacturing by stereolithography is used for printing metals. The metal properties result from analyzing tensile tests first. Subsequently, the real material properties and the best approximation of phenomenologically defined yield criterion is used for optimization. The resulting structures for both an elastic and a plastic optimization are produced and mechanically tested with external loading and supports according to the optimization. The observed stiffness and deformation are analyzed and compared to the simulation results.

Topology and material orientation optimization of layered anisotropic materials

Jantos, Dustin Roman *(Leibniz University Hanover, Germany)* 16:20
Junker, Philipp *(Leibniz University Hanover, Germany)*

Local material properties have significant influence on the structural performance, and should also be optimized besides the structural geometry for high performance applications. Optimized geometries are often hard or even impossible to produce with conventional methods. However, modern additive manufacturing methods allow to produce more complex geometries, also including those resulting from topology optimization. Structures produced with additive manufacturing often inherent anisotropic material properties due to the manufacturing process, i.e. weaker stiffness between layers. But anisotropy can also be exploited purposely due to the high weight to stiffness performance of those materials, as for example fiber reinforced polymers. Thus, the (local) orientation of fibers should be considered to be optimized.

Most additive manufacturing processes yield anisotropic materials with all fibers parallel to a specific, globally defined plane, e.g. the print plane (z-axis) in 3D-Printing. This constraint has to be addressed for an appropriate material orientation optimization. To this end, a method

for simultaneous optimization of the topology and the material orientation based on thermodynamic principles is presented. Within the thermodynamic optimization, the stationary condition of a variational principle derived from material thermodynamics is evaluated to derive (partial) differential equations for the design variables, i.e. the solution of those differential equations serve as update scheme for the optimization. To model layered anisotropic materials, the material orientation is defined by a global layer plane normal and the local orientation of the fibers parallel to the layer plane, which are subject to optimization. The global layer plane normal can be optimized as well or can be prescribed by the user. A filtering technique is presented to constrain the (two-dimensional) maximum fiber curvature within the layers. In addition, the topology is optimized simultaneously by means of a density based approach (SIMP).

After an introduction to the theory of the model, numerical examples are presented in the talk.

Topology optimization considering self-weight

Masarczyk, Daniela *(University of Kassel)* 16:40
Kuhl, Detlef *(University of Kassel)*

In the context of sustainable and resource-efficient construction in civil engineering, the design of optimized structural elements represents a central challenge. Desired structural properties can be achieved or improved by geometrical adaptation of structural elements to the load. This design task is frequently supported by numerical optimization of their shape, their topology or both.

Subject of the present study is the topology optimization with consideration of self-weight. In many applications in civil engineering, self-weight represents the significant load case which can be illustrated by comparison of the self-weight of a bridge to the exterior loading it experiences by traffic. Research on topology optimization excluding self-weight significantly outnumbers research taking it into account.

This study is focused on optimization of structural stiffness with a bound on the disposable amount of material. The Solid Isotropic Material with Penalization (SIMP) method [1] is applied to relax the material distribution problem. The aim to optimize the structural behavior results in a strongly nonlinear optimization problem due to the implicit dependence of structural response on the material distribution. Differing from considerations excluding self-weight, taking it into account results in a non-monotonously decreasing behavior of the objective function with respect to the design variables which represents a challenge for gradient-based optimization [2]. Furthermore, ubiquitous loading by self-weight may result in unconstrained deformation in areas that are occupied by little material.

Due to the nonlinearity of the task, an approximation technique, Sequential Quadratic Programming (SQP) [3] with BFGS-approximation of the Hessian, is applied to numerically solve the optimization problem. Small deformations are considered, the structural analysis is carried out using the Finite Element Method.

[1] M. P. Bendsøe. Optimal shape design as a material distribution problem. *Structural Optimization*, 1(4):193 - 202, 1989.

[2] M. Bruyneel and P. Duysinx. Note on topology optimization of continuum structures including self-weight. *Structural and Multidisciplinary Optimization*, 29(4):245-256, 2005.
[3] K. Schittkowski. On the convergence of a sequential quadratic programming method with an augmented lagrangian line search function. *Mathematische Operationsforschung und Statistik. Series Optimization*, 14(2):197-216, 1983

Influence of weighted gradients in topology optimization of flexible multibody systems

Azari Nejat, Ali *(Hamburg University of Technology)*
Held, Alexander *(Hamburg University of Technology)*
Seifried, Robert *(Hamburg University of Technology)*

17:00

In dynamics, the method of flexible multibody systems is widely used to model and simulate mechanical systems, which undergo large nonlinear motions, including vibrations and deformations. Assuming that the deformations remain small and elastic, the floating frame of reference approach can be utilized for the description of the body deformation with respect to a reference frame, which allows for a separation of the large nonlinear rigid body motion and deformation. In this case, the corresponding deformation is approximated by time-dependent elastic coordinates multiplied by a set of global shape functions, which can, for instance, be obtained from an underlying FE model of the flexible bodies. In other words, the deformation is described by a reduced set of selected elastic coordinates considering only the essential degrees of freedom. Hence, this method reveals high efficiency, although the flexible bodies of the FE models are usually finely discretized to ensure accurate analysis or optimization of flexible multibody systems.

To improve the system performance, for instance, a fully-coupled topology optimization of flexible bodies can be performed, where a semi-analytical adjoint sensitivity analysis provides the required exact gradient. However, the calculation of the exact gradient by the adjoint sensitivity analysis is time-consuming since, among others, the derivatives of the system matrices with respect to the design variables have to be computed. Therefore, to reduce the number of required design variables, in this work, a level set-based topology optimization is considered, where in each iteration, the boundaries between void and solid areas are well defined by an implicit level set function, and the gradient calculation for empty elements can be skipped. Moreover, a modified Solid Isotropic Material with Penalization (SIMP) method is used, in which the parameterization of the stiffnesses and masses of the finite elements is adapted such that numerical issues in the model reduction are omitted. However, it turns out that in the optimization of dynamic systems, the weighting of the stiffness and mass has an influence on the gradient and hence the optimization results. Therefore, SIMP approaches with different weights are tested within the developed level set-based topology optimization procedure to check the validity of the chosen SIMP parameterization strategy. As an application example, a flexible piston rod in a slider-crank mechanism is optimized. The obtained results show, among others, the range of appropriate weightings in the studied example.

Isogeometric topology optimization using the Cahn-Hilliard based phase-field method

Kikis, Georgia *(Lehrstuhl für Baustatik und Baudynamik, RWTH Aachen, Germany)*
Klinkel, Sven *(Lehrstuhl für Baustatik und Baudynamik, RWTH Aachen, Germany)* 17:20

Topology optimization that has been widely used in aerospace and mechanical engineering has found its way into civil engineering and enables the creation of lightweight structures with an optimal load-carrying behavior. In this contribution, the phase-field method is used to compute the optimal material distribution of a structure in order to minimize its compliance and, thus, maximize its stiffness. The phase-field method can naturally describe the formation of holes and topological changes. It is based on the Cahn-Hilliard equation that directly satisfies the mass conservation condition. The optimal topology is defined as the steady state of the phase transition which minimizes the penalized objective functional and, thus, avoids the need for an optimizer. Isogeometric analysis is applied to describe the geometry and the material distribution of the structure. It allows for an exact representation of the geometry, the material and void regions of the optimized structure and unifies the design and analysis process. Several examples are studied in order to investigate the accuracy and efficiency of the method. The optimized topology is compared to the results obtained with an isogeometric topology optimization method using the SIMP approach in order to highlight the differences of these two methods.

Topology Optimization Using the Phase Field Method and Compliance Constraints

Fohler, Fabian *(Brandenburgische Technische Universität Cottbus-Senftenberg, Germany)*
Dornisch, Wolfgang *(Brandenburgische Technische Universität Cottbus-Senftenberg, Germany)* 17:40

This work focuses on topology optimization by using a phase field variable for describing the distribution of material in a design space. This is very advantageous since the boundary between material and void does not need to be tracked. The objective function, which can be included directly in the potential formulation, also avoids the use of a separate sensitivity analysis. The entire calculation and development of the phase field is done in finite element analysis. Another advantage of the phase field formulation is the possibility to create new voids within existing material areas or to make existing voids disappear without the need for separate algorithms. Overall, this eliminates the major disadvantages of other optimization methods such as SIMP or Level-Set. The phase field method was originally developed to describe phase transitions, for example in the process of steel hardening. The seminal works come from Allen, Cahn and Hilliard. The first links between the phase field approach and topology optimization go back to Bourdin and Chambolle. The Ginzburg-Landau energy is used to force the domain into one of the two phases (material or void) and only allows a thin transition zone. Furthermore, the Allen-Cahn equation serves to describe the phase field evolution within an artificially introduced time. Without this reaction-diffusion equation, finding an optimized state based on a random initial domain would hardly be possible. Within this

framework two different objective functions with related constraints are incorporated to obtain two varying models. The first was developed by Münch, Gierden and Wagner and uses the homogenization of the equivalent stress, which is somehow similar to maximizing stiffness. The conservation of mass is achieved implicitly by coupling the desired filling level to the limit value of the equivalent stress. The second model is based on a compliance constraint, so the overall mass in the design space is to be minimized. Both objectives are well known in structural mechanics but in practical application the minimization of the mass is more often of interest. We show the development of the phase field for a benchmark example with both models and the associated change in the potentials. Comparing the results of both models also proves that they perform equally well. We further investigate the impact of the numerical parameters on the complexity of the final topologies.

Eigenvalue Optimization with a Phase Field Approach

Garcke, Harald *(University of Regensburg)*
Hüttl, Paul *(University of Regensburg)*
Kahle, Christian *(University of Koblenz)*
Knopf, Patrik *(University of Regensburg)*
Laux, Tim *(University of Bonn)*

18:00

We investigate the problem of finding optimal domains for physical systems. Thus we search for optimal domains in which these systems are satisfied, such that some objective, depending on the system and thus especially on its domain, is minimized. Choosing a hold-all domain Ω we describe the distribution of void and domain of interest by the values of a phase field function. In a first step we derive and analyse appropriate formulations to obtain model equations that are posed on the hold-all domain. This results in a phase field variable $\varphi \in H^1(\Omega) \cup L^\infty(\Omega)$ that encodes the domain of interest by $\varphi(x)=1$ and the void domain by $\varphi(x) = -1$. As a result, the saught domain is encoded by a function and concepts from optimization with PDE constraints can be used. Due to the regularity of the optimization variable φ, we apply the variable metric projection type method proposed in [L. Blank and C. Rupprecht, SICON 2017, 55(3)]. Examples include eigenvalue optimization for diffusion and linear elasticity equation.

S16-05: Optimisation

Date: June 2, 2023 08:30-10:30
Room: HSZ/105

Multi-objective Optimization for Neural Networks Training: Weighted Chebyshev Scalarization

Hotegni, Sedjro Salomon *(Paderborn University, Germany)* 08:30
Peitz, Sebastian *(Paderborn University, Germany)*
Berkemeier, Manuel *(Paderborn University, Germany)*

Multi-objective optimization has been an active area of research in the field of optimization and machine learning. In the context of neural networks training, traditional optimization algorithms have primarily focused on minimizing a single objective function, such as the mean squared error or cross-entropy loss. While this approach has been successful in many applications, it can lead to suboptimal solutions when multiple objectives are relevant to the prediction task. In this case, there can be optimal trade-offs between the objectives, which form the Pareto-Front.

A wide range of techniques have been developed to address multi-objective optimization problems, including evolutionary algorithms, heuristics, and gradient-based methods. However, these techniques can be computationally expensive, especially for large-scale problems. In these cases, scalarization approaches, which map the multiple objectives to a single scalar value, might be preferable. These approaches allow for the simultaneous optimization of multiple objectives by considering their trade-offs in a single function.

The Weighted Chebyshev Scalarization (WCS) approach, which is the focus of this work, is one such scalarization method that has been used in a variety of applications. In our setting, it is equivalent to the well-known Pascoletti-Serafini scalarization and allows for the encoding of user preferences in the scalarization of the multi-objective optimization problem by varying a weight vector and a reference point. It then becomes possible to use existing single-objective optimization algorithms to train and obtain highly accurate predictions. Moreover, WCS also work for non-convex Pareto-Fronts, whereas more simple scalarization formulas do not.

Our experience is based on a classification problem and our objective has been to simultaneously optimize two loss functions: Cross-entropy loss and Kullback-Leibler divergence loss. The cross-entropy loss encourages the classifier to have high confidence in its predictions, and the KL divergence loss ensures that it doesn't overestimate the probability of a class. The constrained optimization problem resulting from applying WCS was solved with the Augmented Lagrangian approach, combined with Adam Optimizer. The proposed approach was evaluated using the MNIST dataset and we compared two convergence approaches: focusing on the convergence of the Augmented Lagrangian minimization process and the convergence of the Adam Optimization process.

For a fixed weight vector and a fixed reference point, our results indicate that focusing on the convergence of the Augmented Lagrangian minimization process leads to better accuracy (>96%) compared to focusing on the convergence of the Adam Optimization process (<77%). Further, by varying the weights, we found that the best performance of the model in terms of accuracy was obtained when the cross-entropy loss was given more importance

than the KL divergence loss. In summary, in this work, the importance of considering multiple relevant objectives in the optimization process for neural network training is highlighted and the Weighted Chebyshev Scalarization approach is shown to be a promising solution to this problem.

Nonlinear Conjugate Gradient Directions with Guaranteed Descent for Smooth Multi-Objective Optimization

Berkemeier, Manuel Bastian *(Paderborn University, Germany)*
Peitz, Sebastian *(Paderborn University, Germany)*
08:50

In single-objective optimization, the use of nonlinear conjugate gradient directions is known to improve the convergence behavior of iterative first-order methods compared to simple steepest descent when applied to nonlinear problems. Without requiring second derivatives, these methods can often traverse flat valleys near local minima. The theory for popular CG coefficients often requires Wolfe conditions to be satisfied by (inexact) line-search procedures.

This is also the case for the known generalizations of some popular CG coefficients, such as Fletcher-Reeves, Polak-Ribière, Hestenes-Stiefel, or Dai-Yuan, in the multi-objective setting [1]. Now, enforcing Wolfe conditions makes line-search more difficult and might be prohibitive in some situations, e.g., if the evaluation of gradients is expensive or if there are constraints.

That is why we present some coefficients inspired by the idea of guaranteed descent in single-objective optimization. These new CG schemes ensure that a criticality measure at the next iterate can be related to the steepest descent direction — independent of the actual line-search procedure! We are thus able to easily establish lim-inf convergence results for an algorithm using a simple Armijo-like backtracking. Additionally, numerical experiments show that indeed, these new directions can handle flat valleys much better than the multi-objective steepest descent direction, at very little additional cost.

[1] L. R. Lucambio Pérez and L. F. Prudente, "Nonlinear Conjugate Gradient Methods for Vector Optimization," SIAM J. Optim., vol. 28, no. 3, pp. 2690-2720, Jan. 2018, https://doi.org/10.1137/17M1126588.

Generating the Pareto-frontier in multi-objective optimization problems by a design of experiments based on the Normal-boundary-intersection method – Applying optimization methods to test plans for process optimization

Gellerich, Peter Anton *(Institute for Natural Materials Technology, Technische Universität Dresden, 01069 Dresden, Germany; Uhlmann Pac-Systeme GmbH & Co. KG, 88471 Laupheim, Germany)*
Majschak, Jens-Peter *(Institute for Natural Materials Technology, Technische Universität Dresden, 01069 Dresden, Germany)*
09:10

Finding the optimum process parameters for manufacturing processes is an important issue in industrial production. However, for most processes there is no mathematical model available to provide the necessary objective function of the optimization problem. In this case, experiments may either quantify an explicit model in advance, or provide empirical data while executing the optimization algorithm.

This paper contributes to the last approach, and covers multi-objective optimization problems with unknown objective functions, which can neither solved analytically nor computed numerically. In order to generate the Pareto-frontier of such a problem, experiments may be executed. The paper shows, how to develop a design of experiments based on the Normal-boundary-intersection method, and how to generate the Pareto-frontier by executing experiments according to the test plan. It addresses the specific requirements to optimization methods for use in test plans, and discusses the practical limitations due to solving an optimization problem by experiments.

The design of experiments is verified by using a case study on heat sealing in industrial packaging of consumer goods. The behavior of the method towards discrete and binary objectives and constraints is discussed regarding the results of the case study.

Gradient-based determination of principal design influences on composite structures

Liedmann, Jan *(TU Dortmund, Germany)* 09:30
Barthold, Franz-Joseph *(TU Dortmund, Germany)*
Gerzen, Nikolai *(Technische Hochschule Ostwestfalen-Lippe, Germany)*

Optimization of fiber-reinforced composite structures with nonlinear load-bearing behavior is a complex task that is becoming increasingly relevant in practice. Therefore, it is desirable to automatically determine essential influences on the structural behavior of fiber composite shells and stability-relevant objective functions and constraints in the context of structural optimization. This work deals with a variational approach for the derivation and computation of design sensitivities of elastic solid shell structures, as described in [1], and the extension to anisotropic layered composite structures. Design sensitivities concerning fiber angles and layer thicknesses are derived and quantitatively determined in the context of the finite element method (FEM). The anisotropic analysis model is founded on [2], in which a sophisticated solid-shell formulation based on reduced integration, as described in [3], is extended to discretize the composite with only one element over the whole thickness by means of multiple integration points. This can be understood as a special case of equivalent-single-layer theories (ESLT). Examination of global stiffness and sensitivity matrices using methods from principal component analysis (PCA), such as singular value decomposition (SVD), are used to identify crucial design changes corresponding to major changes in the structural behavior of the composite. Results are discussed by referecne to a chosen numerical example.

[1] N. Gerzen, et al. Variational sensitivity analysis of a non-linear solid shell element. International Journal for Numerical Methods in Engineering 96(1), 29-42, 2013.
[2] O. Barfusz, R. Smeenk, S. Reese. Solid-Shells based on reduced integration - Geometrically non-linear analysis of layered structures. ECCM6 / ECFD 7 Glasgow, 2018.
[3] S. Klinkel, F. Gruttmann, W. Wagner. A continuum based three-dimensional shell element for laminated structures. Computers and Structures 71, 43-62, 1999.

Shape modes of dynamic structures

Ghasemi, Seyed Ali *(TU Dortmund University, Germany)*
Liedmann, Jan *(TU Dortmund University, Germany)*
Barthold, Franz-Joseph *(TU Dortmund University, Germany)*

09:50

This work aims to gain a deeper understanding of sensitivity information through the use of principal component analysis (PCA). By decomposing sensitivity matrices, it is possible to explore and analyze the underlying relationships between variables and the impact of their changes on the overall structure. The approach for this analysis is discussed in [1]. PCA allows us to analyze the eigenvectors of the covariance matrix, which are known as the principal components. The first principal component is considered the most significant mode of variation as it indicates the direction with the highest variance in the data. Similarly, the second principal component represents the direction with maximum variance, but this time it must be orthogonal to the first principal component. This process continues for the remaining principal components. The work at hand makes use of gradient-based sensitivity analysis [2] for dynamic structures and compares two different methods for shape design: Isogeometric Analysis (IGA) [3] and Finite Element Method (FEM). The main focus is on using direct differentiation, but if analytical gradients are not available, numerical differentiation methods such as complex-step method (CSM) and automatic differentiation (AD) can be used as alternatives. We utilize different types of basis functions, such as Bernstein polynomials, B-Splines, and Non-Uniform Rational B-Splines (NURBS), to describe the shape of the structure. IGA has several advantages over traditional FEM-based approaches. These advantages include the ability to accurately describe geometry using fewer control points, high-order continuity, and increased flexibility due to control point weights. These characteristics have a significant impact on shape sensitivity analysis. IGA is used during the structural optimization process to avoid costly remeshing and design velocity field calculations. It is more efficient and effective than traditional FEM approaches for these tasks. In contrast to static analysis, the response of a structure to time-dependent loads is significantly affected by inertia and damping effects. The necessary computational characteristics for this type of problem are discussed and the full solution algorithm is presented.

References

[1] N. Gerzen and F.-J. Barthold, “Design space exploration based on variational sensitivity analysis,” PAMM, vol. 14, no. 1, pp. 783-784, Dec. 2014. https://doi.org/10.1002/pamm.201410374.

[2] F.-J. Barthold, N. Gerzen, W. Kijanski, and D. Materna, “Efficient variational design sensitivity analysis,” in Mathematical Modeling and Optimization of Complex Structures (Computational Methods in Applied Sciences), P. Neittaanmäki, S. Repin, and T. Tuovinen, Eds., Computational Methods in Applied Sciences. Switzerland: Springer International Publishing, 2016, vol. 40, ch. Efficient Variational Design Sensitivity Analysis. https://doi.org/10.1007/978-3-319-23564-6_14.

[3] T. Hughes, J. Cottrell, and Y. Bazilevs, “Isogeometric analysis: Cad, finite elements, nurbs, exact geometry and mesh refinement,” Computer Methods in Applied Mechanics and Engineering, vol. 194, no. 39-41, pp. 4135-4195, 2005. https://doi.org/10.1016/j.cma.2004.10.008.

S17: Applied and numerical linear algebra

Organizer(s): **Mach, Thomas** *(U Potsdam)*
Ullmann, Elisabeth *(TU München)*

S17-01: Applied and numerical linear algebra

Date: May 31, 2023 08:30-09:30
Room: HSZ/103

Randomized sketching of nonlinear eigenvalue problems and beyond

Güttel, Stefan *(The University of Manchester)* 08:30
Kressner, Daniel *(EPFL)*
Vandereycken, Bart *(University of Geneva)*

Rational approximation is a powerful tool to obtain accurate surrogates for nonlinear functions that are easy to evaluate and linearize. The interpolatory adaptive Antoulas-Anderson (AAA) method is one approach to construct such approximants numerically. For large-scale vector- and matrix-valued functions, however, the direct application of the set-valued variant of AAA becomes inefficient. We propose and analyze a new sketching approach for such functions called sketch AAA that, with high probability, leads to much better approximants than previously suggested approaches while retaining efficiency. The sketching approach works in a black-box fashion where only evaluations of the nonlinear function at sampling points are needed. Numerical tests with nonlinear eigenvalue problems illustrate the efficacy of our approach, with speedups above 200 for sampling large-scale black-box functions without sacrificing on accuracy.

Divide and conquer methods for functions of matrices with banded or hierarchical low-rank structure

Cortinovis, Alice *(Stanford University, United States of America)* 09:10
Kressner, Daniel *(EPFL Lausanne, Switzerland)*
Massei, Stefano *(University of Pisa, Italy)*

This talk is concerned with approximating matrix functions for banded matrices, hierarchically semiseparable matrices, and related structures. We propose new divide-and-conquer methods which exploit the fact that these matrices can be (recursively) decomposed as a sum A = D + R of a block diagonal matrix D and a low-rank correction R. While the update f(A) - f(D) often has low numerical rank and can be approximated via (rational) Krylov subspace projections, the block diagonal part f(D) is computed recursively for each diagonal block. We present a convergence analysis that relates the accuracy attained by the algorithm with the best polynomial or rational approximations of the function. For the special case of a banded matrix, we show that the divide-and-conquer method reduces to a much simpler algorithm, which proceeds by computing matrix functions of small submatrices of A. When only the trace or the diagonal of the matrix function is of interest, we demonstrate - in practice and in theory - that convergence can be faster. Finally, we test the algorithms on a variety of matrices and functions; the numerical results demonstrate that, most of the time, the proposed methods

outperform state-of-art techniques with respect to time consumption and offer a comparable accuracy.

S17-02: Applied and numerical linear algebra

Date: June 1, 2023 16:00-19:00
Room: HSZ/103

On a new family of low-rank algorithms for large-scale algebraic Riccati equations

Faßbender, Heike *(TU Braunschweig, Germany)* 16:00
Bertram, Christian *(TU Braunschweig, Germany)*

Finding the unique stabilizing solution $X = X^H$ of a large-scale continuous-time algebraic Riccati equation (CARE) $0 = R(X) := A^HX + XA + C^HC - XBB^HX$ with a large, sparse n-x-n matrix A, an n-x-m matrix B and an p-x-n matrix C is of interest in a number of applications. Here, B and C^H are assumed to have full column and row rank, resp., with m, p « n. The unique stabilizing solution $X = X^H$ is positive semidefinite and makes the closed-loop matrix $A-BB^HX$ stable. Even so A is large and sparse, the solution X will still be a dense matrix in general. But our assumptions on B and C often imply that the sought-after solution X will have a low numerical rank (that is, its rank is « n). This allows for the construction of iterative methods that approximate X with a series of low rank matrices stored in low-rank factored form. To be precise, we focus on Hermitian low-rank approximations X_j to X of the form $X_j = Z_jY_jZ^H$, where Z_j is an n-x-k_j matrix with only few columns and Y_j is a small square k_j-x-k_j Hermitian matrix. There are several methods which produce such a low-rank approximation. Our approach is based on a block rational Arnoldi decomposition and an associated block rational Krylov subspace spanned by A^H and C^H. The approximations X_j as well as $||R(X_j)||_F$ can be computed fast and efficiently. In particular, our approach gives a whole new family of algorithmic descriptions of the same approximation sequence X_j to the Riccati solution as four other algorithms for CARE previously known in the literature. A new feature of the family of algorithms, useful for efficient implementation, is that it allows shifts to be added to the solution not just one at a time, but several at a time. The linear systems of equations of the form $(A^H+\sigma_j)V = C^H$ to be solved for this purpose can be solved simultaneously. The focus of the talk will be on the theoretic background of the family of algorithms rather than on a comparison with other known algorithms.

Symplectic Exponential Runge-Kutta-Methods for Solving Large Nonlinear Hamiltonian Systems

Peters, Till *(Technische Universität Braunschweig, Germany)* 16:40

We study stiff Hamiltonian systems of the form

$y'(t) = My(t) + f(y(t)), y(t\_0) = y\_0, t \in [t\_0, T]$ (1)

with a Hamiltonian matrix $M \in R^{2d\times 2d}$ and a suitable function f: $R^{2d} \to R^{2d}$. Here M is called Hamiltonian if M fulfills $(JM)^T = JM$ with the matrix J = [0_d, I_d; -I_d, 0_d]. Moreover, M forms the main part of the stiffness in system (1) by having only eigenvalues on the imaginary axis with large magnitude. Exponential integrators are known to be useful for integrating stiff systems (1). These integrate the linear part of the differential equation exactly which can help to weaken the stiffness of the differential equation. Symplectic methods are suitable

for integrating Hamiltonian systems because they preserve the symplectic flow of the system and provide good long-term results (see also [1]). Combining these two aspects, Mei and Wu show in [2] starting from symplectic Runge-Kutta-Methods how to generate symplectic exponential Runge-Kutta-Methods. For large dimensions d, the evaluation of the action of a matrix exponential on a vector is costly. A standard approach to reduce these costs is the use of Krylov subspace methods to approximate the matrix-vector-products of the form $e^M b$ with $M \in \mathrm{R}^{2d\times 2d}$ and $b \in \mathrm{R}^{2d}$. We investigate different Krylov subspace methods such as the standard Arnoldi method or different symplectic methods like the symplectic Lanczos method. Furthermore, we compare resulting approximative integrators in terms of accuracy in the matrix exponential approximation, accuracy in solving the system and preservation of the Hamiltonian structure.

References

[1] E. Hairer, C. Lubich, and G. Wanner. Geometric Numerical Integration. Springer-Verlag Berlin Heidelberg New York, second edition, 2006.

[2] L. Mei and X. Wu. Symplectic exponential Runge-Kutta-methods for solving nonlinear Hamiltonian systems. Journal of Computational Physics, 338:567584, 2017.

Data-driven Loewner matrix approach for estimating large-scale structured real stability radius

Aliyev, Nicat *(Czech Technical University, Czech Republic)* 17:00

The autonomous linear dynamical system $x' = Ax$, with $A \in \mathrm{R}^{n\times n}$ is asymptotically stable, if all of the eigenvalues of A lie in the open left-half of the complex plane. Here, matrix A is said to be Hurwitz stable, or in short, a stable matrix. In practice, the stability of a system can be infringed due to perturbations or modeling errors. The previous system is said to be robustly stable if the system, as well as all of its perturbations from a certain perturbation class, are stable. To measure the robustness of the system subject to perturbations, a quantity of interest is the stability radius, or in other words, the distance to instability. In this work we propose a method based on the Loewner matrix framework to estimate the structured real stability radius in an efficient way. We prove that the proposed method converges, in theory, at a quadratic rate. The quadratic convergence of the method is due to Hermite interpolation properties between the transfer functions of the full and reduced problems. Hence, it efficiently/accurately estimates the structured real stability radius for large-scale cases. The method is illustrated on several examples.

Learning Structure-preserving Quadratic Models of Hamiltonian Systems

Yıldız, Süleyman *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Goyal, Pawan *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Bendokat, Thomas *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Benner, Peter *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany; Otto von Guericke University, Germany)*

17:20

Model order reduction of Hamiltonian systems needs to preserve the intrinsic symplectic structure of the given problem for the reduced-order model to stay reasonably accurate over longer time.
For this, the proper symplectic decomposition (PSD) of the given data can be approximated, and the reduced-order model can be found via projection onto a symplectic subspace.
In case of a non-linear Hamiltonian function, further hyperreduction methods like symplectic DEIM can be used to achieve efficient computability of the reduced-order model.
As an alternative, we study the modelling of Hamiltonian systems with cubic Hamiltonian functions, resulting in quadratic dynamics of the reduced-order model.
Given generalized position and momentum data of a dynamical system, the studied method learns symmetric tensors for the low dimensional quadratic dynamics, enforcing the Hamiltonian structure, in combination with a symplectic auto-encoder.
The enforced Hamiltonian structure yields long-term accuracy of the model, while the cubic Hamiltonian function provides relatively low model complexity.
In that way, the symplectic structure is inferred from the data for a non-linear underlying Hamiltonian function, and the reduced-order model can be computed efficiently.

A Novel Recycling Linear Solver for Stable Parametric Model Order Reduction

Ahuja, Kapil *(Indian Institute of Technology Indore, India)*
Choudhary, Rajendra *(Pandit Deendayal Energy University, Gandhinagar, India)*

17:40

We study stability of a interpolatory model order reduction (MOR) algorithm for parametric linear dynamical systems with respect to inexact linear solves, that is, the IPMOR algorithm. This analysis is easily extendible to other MOR algorithms for such systems. Besides deriving the two conditions for stability, accuracy expression, and subsequent experimentation, our most novel contribution here is achieving a backward stable IPMOR. To achieve this, we first categorize the involved orthogonality conditions into different classes. Second, we adapt the underlying linear solver (here BiConjugate Gradient or BiCG) to satisfy these orthogonalities. Finally, and third, we derive a new variant of the Recycling BiCG so that these orthogonalities can be achieved with no code changes to the linear solver (for a end user or a model reducer here) as well as cheaply (extra orthogonality cost offset by savings because of recycling).

Damping optimization of mechanical systems using a singe damper

Truhar, Ninoslav *(University of Osijek, Osijek, Croatia)* 18:20
Weber, Wolfgang E. *(Helmut Schmidt University, Hamburg, Germany)*
Veselić, Krešimir *(Fernuniversitat Hagen, Hagen, Germany)*

In this talk, we address the problem of optimal placement of a damper based on the two different optimization criteria for optimal damping of multi-body oscillators with arbitrary n degrees of freedom. We consider the average total energy and the average total displacements. For these criteria, we have shown that the optimal position of a single damper does not depend on the respective criterion but on the specific position of the single masses of the multi-body oscillator. The novelty of our results includes a standardized formulation and a simple example illustrating the application of both criteria and the optimal damping of a vibration chain with arbitrary n degrees of freedom by one single damper. Further, since the damping optimization by means of the aforementioned optimization criteria is not a straightforward task, a numerical approach using the closed formula is also presented. This approach can be used for efficiently calculating optimal damping for medium-size problems with $n \leq O(10^4)$.

Solving the Parametric Eigenvalue Problem by Taylor Series and Chebyshev Expansion

Mach, Thomas *(University of Potsdam, Institute of Mathematics, Germany)* 18:40
Freitag, Melina A. *(University of Potsdam, Institute of Mathematics, Germany)*

We discuss two approaches to solving the parametric (or stochastic) eigenvalue problem $A(\mu)\lambda(\mu)=A(\mu)v(\mu)$. One of them uses a Taylor series expansion and the other a Chebyshev expansion. The parametric eigenvalue problem assumes that the matrix A depends on a parameter μ, where μ is real and might be a random variable. Consequently, the eigenvalues and eigenvectors are also functions of μ. Parametric eigenvalue problems occur in different applications, for instance when Hadamard matrix functions are used, for PDEs with unknown material constants, or in conjunction with matrix-value ODEs.

We compute a Taylor approximation of these functions about μ_o by iteratively computing the Taylor coefficients. The complexity of this approach is $O(n^3)$ for all eigenpairs, if the derivatives of $A(\mu)$ at μ_o are given. The Chebyshev expansion works similarly. We first find an initial approximation iteratively which we then refine with Newton's method. This second method is more expensive but provides a good approximation over the whole interval of the expansion instead around a single point.

We present numerical experiments confirming the complexity and demonstrating that the approaches are capable of tracking eigenvalues at intersection points. Further experiments shed light on the limitations of the Taylor expansion approach with respect to the distance from the expansion point μ_o.

S17-03: Applied and numerical linear algebra

Date: June 2, 2023 16:00-18:00
Room: HSZ/103

Multigrid methods for block Toeplitz and block circulant matrices

Bolten, Matthias *(Bergische Universität Wuppertal, Germany)* 16:00
Donatelli, Marco *(Università dell'Insubria, Italy)*
Ferrari, Paola *(Bergische Universität Wuppertal, Germany)*
Furci, Isabella *(Bergische Universität Wuppertal, Germany)*

Multigrid methods for Toeplitz matrices and circulant matrices are well understood and in many cases are optimal solvers. Examples include matrices arising from the discretization of scalar partial differential equations with constant coefficients. Moreover, these results carry over to matrices that are not Toeplitz or circulant by means of the theory of generalized locally Toeplitz matrices.

For certain discretization schemes, like higher order finite elements, or systems of PDEs the analysis techniques used are not appropriate, as the matrices do have block Toeplitz or block circulant structure or perturbations thereof. We analyzed these cases and extended the existing theory, providing sufficient conditions for convergence of twogrid methods for these systems. We obtained results for block Toeplitz and block circulant matrices with blocks as they appear in the higher-order finite element setting as well as for those with blocks as they appear in systems with saddle point structure. In the first case we were also able to proof convergence of the V-cycle in multigrid methods.

Properties of hybrid LSQR method for the solution discrete inverse problems in Single Particle Analysis

Havelková, Eva *(Faculty of Mathematics and Physics, Charles University, Czech Republic)* 16:20
Hnětynková, Iveta *(Faculty of Mathematics and Physics, Charles University, Czech Republic)*

In this contribution, we focus on properties of hybrid LSQR method applied to the solution of discrete inverse problems $Ax \sim b$ arising in single particle analysis. Hybrid LSQR represents a combination of iterative projection by Golub-Kahan bidiagonalization with Tikhonov regularization applied to the projected problem. Such a combination has shown to be efficient in prevention of over-fitting of the computed approximation while maintaining the computational cost feasible. Properties of the algorithm are, however, highly dependent on the choice of regularization parameters. Here, we describe suitable choices of regularization parameters for hybrid LSQR motivated by the underlying application. Further, we analyze the resulting properties of the projected problem, its solution and residual vectors, and compare them to the properties of standard LSQR. Numerical experiments performed on realistic data will be used for demonstration.

Hierarchical Block Structures for the Preconditioning of Saddle Point Problems with H-Matrix Decompositions

Grams, Jonas *(Hamburg University of Technology, Germany)* 16:40
Le Borne, Sabine *(Hamburg University of Technology, Germany)*

Fluid flow problems can be modelled by the Navier-Stokes, or Oseen equations. Their discretization results in saddle point problems. These systems of equations are typically very large and need to be solved iteratively. Standard (block-) preconditioning techniques for saddle point problems rely on an approximation of the Schur complement. Such an approximation can be obtained by a hierarchical matrix (H-Matrix) LU-decomposition for which the Schur complement is computed explicitly. The computational complexity of this computation depends, among other things, on the hierarchical block structure of the involved matrices. However, widely used techniques do not consider the connection between the discretization grids for the velocity field and the pressure, respectively. Thus, a problem dependent hierarchical block structure for the FEM discretization of the gradient operator is presented. The block structure of the corresponding saddle point matrix block is improved by considering the connection between the two involved grids.Numerical results will show that the improved block structure allows for a faster computation of the Schur complement, the bottleneck for the set-up of the H-Matrix LU-decomposition.

Fully reliable iteration method based on simplification of the original operator

Samrowski, Tatiana S. *(Universität Zürich, Switzerland)* 17:00

We consider an iteration method for solving the problem $Au = f$ with a complicated positive definite operator A by means of a simpler operator A_0 (which inversion is much cheaper than inversion of A). The difference between A and A_0 is controlled by the parameter δ. We prove contraction of the iteration operator and deduce fully computable two-sided a posteriori estimates.

Symbol-Based Analysis of Structured Matrices in Electromagnetic Scattering Problems

Bolten, Matthias *(Bergische Universität Wuppertal, Germany)* 17:20
Furci, Isabella *(Bergische Universität Wuppertal, Germany)*
Spoerer, René *(Bergische Universität Wuppertal, Germany)*

We present a symbol-based analysis of the block-Toeplitz and block-cirulant matrices that arise in the computation of electromagnetic scattering in bounded cavities. This matrix structure occurs when discretising the problem using Nédélec finite elements on a structured grid and can be represented by a matrix-valued generating symbol. The generating symbol is a function which allows the analysis of the asymptotic spectral properties of the matrices [1] and can guide the design of multigrid solvers for the problem [2]. Within this framework, we also interpret the two-step hybrid smoother used in the multigrid method developed by R. Hiptmair for the presented equations [3]. This new frame of reference paves the way for future progress in the optimisation and symbol-based convergence analysis of multigrid solvers for this family of problems.

[1] G. Barbarino, C. Garoni, and S. Serra-Capizzano. Block generalized locally Toeplitz sequences: theory and applications in the multidimensional case. Electron. Trans. Numer. Anal. 53 (2020), 113–216.
[2] M. Bolten, M. Donatelli, P. Ferrari, and I. Furci. A symbol-based analysis for multigrid methods for block-circulant and block-Toeplitz systems. SIAM J. Matrix Anal. Appl. 43 (2022), no. 1, 405–438.
[3] R. Hiptmair. Multigrid method for Maxwell's equations. SIAM J. Numer. Anal. 36 (1999), no. 1, 204–225.

Krylov-Simplex and residual subspace Simplex

Vanroose, Wim I *(U Antwerpen, Belgium)*
Symoens, Bas *(U Antwerpen, Belgium)* 17:40

The Krylov-Simplex iterative method combines Krylov and simplex iterations to minimize the residual r=b−Ax in the max-norm. We search for an optimal solution x_k in a Krylov subspace. A specialized simplex algorithm solves this projected problem and finds the optimal linear combination of Krylov basis vectors to approximate the solution. The resulting simplex algorithm requires the solution of a series of small dense linear systems that only differ by rank-one updates. The QR factorization of these matrices is updated each iteration.

In the Residual subspace simplex method we solve a linear programming problem by projecting the constraints on the space of residuals. This gives a sequence of projected LP problems that are solved with a warm-started dual simplex iteration. Resulting a efficient method to solve large scale LPs with sparse constraint matrices.

S18: Numerical methods for differential equations

Organizer(s): **Gräßle, Carmen** *(TU Braunschweig)*
Maier, Roland *(U Jena)*

S18-01: Numerical methods for differential equations

Date: May 30, 2023 13:30-16:10
Room: HSZ/H02

Certified and Adaptive Surrogate Modeling for Parameterized Large Scale Systems

Ohlberger, Mario *(University of Münster, Germany)* 13:30

Model order reduction for parameterized systems has gained a lot of attention in the last two decades. In this talk we will focus on projection based model order reduction and their efficient application to solve parameterized large scale PDE systems, in particular in the context of PDE constrained optimization problems. We will discuss learning strategies, such as adaptive enrichment as well as a combination of reduced order models with machine learning approaches in the context of time dependent problems. Concepts of rigorous certification and convergence will be presented, as well as numerical experiments that demonstrate the efficiency of the proposed approaches.

Model order reduction for a parametrized Cahn-Hilliard problem

Burkovska, Olena *(Oak Ridge National Laboratory)* 14:10
Gräßle, Carmen *(TU Braunschweig, Germany)*

In this talk, we consider a parametrized Cahn-Hilliard model, where the parameter can appear, e.g., in the initial condition or in the model equations. High-fidelity numerical simulations for different parameter configurations would require a large computational effort. In order to alleviate the computational costs, we utilize a reduced-order technique based on a POD-greedy approach in order to construct a low-dimensional surrogate model. We investigate different potential energies including a smooth double-well and a non-smooth double-obstacle potential. Numerical examples illustrate the approach.

Discretization of PDEs with Variable Coefficients Using Locally Adaptive Sparse Grids

Scherner-Grießhammer, Riccarda *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)* 14:30
Pflaum, Christoph *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*

Elliptic partial differential equations with variable coefficients can be discretized on sparse grids. With prewavelets being L^2-orthogonal, one can apply the Ritz-Galerkin discretization to obtain a linear equation system with $O(N(\log(N))^{d-1})$ unknowns. However, for several applications like PDEs with corner singularities or the high-dimensional Schrödinger equation locally adaptive grids are needed to obtain optimal convergence. Therefore, we introduce a new kind of locally adaptive sparse grid and a corresponding algorithm that allows solving the resulting finite element discretization equation with optimal complexity. These grids are

constructed by local tensor product grids to generate adaptivity but still maintain a local unidirectional approach. To obtain an efficient implementation of the algorithm, new approaches to data structures are needed. These are, for example, global hashtables and depth-dependent hashtables. There are several options to parallelize the corresponding matrix-vector multiplication. One of these is splitting the algorithm by 2^d cases of restrictions and prolongations. Another is the usage of the local tensor product grid. That allows both MPI and OpenMP parallelization.

Higher order space-time finite element multigrid solver for coupled hyperbolic-parabolic systems

Bause, Markus *(Helmut Schmidt University Hamburg, Germany)* 14:50
Anselmann, Mathias *(Helmut Schmidt University Hamburg, Germany)*

Space-time finite element methods (STFEMS) allow the natural construction of higher order discretizations to systems of flow and multi-physics [M. Bause, A. Anselmann, U. Köcher, F. A. Radu, Convergence of a continuous Galerkin method for hyperbolic-parabolic systems, Comput. Math. with Appl., submitted (2022), pp. 1–24; https://arxiv.org/abs/2201.12014.]. They offer the potential to achieve accurate results on computationally feasible grids with a minimum of numerical costs. However, constructing higher order numerical methods maintaining stability and inheriting most of the rich structure of the continuous problem becomes increasingly difficult. Further, to realize higher order schemes that require less CPU time for achieving comparable accuracy, also solvers of optimal complexity, are necessary [M. Anselmann, M. Bause, A geometric multigrid method for space-time finite element discretizations of the Navier-Stokes equations and its application to 3d flow simulation, ACM Trans. Math. Softw., submitted (2021), pp. 1–27; https://arxiv.org/abs/2111.12505 1]. Ideally, the approach should also offer robustness with respect to the physical (model) parameters. We present and analyze corresponding solution techniques for coupled systems of hyperbolic and parabolic equations modeling, for instance, fully dynamic poro- and thermoelastic phenomena in material and natural sciences. The accurate resolution of poroelastic wave propagation argues for higher order space and time discretizations. **Tailored STFEMs** are suggested. **Optimal order error estimates** are presented for these families of schmes. **Two-field** and **structure-preserving multi-field STFEMs** are discussed. Their potential to preserve conservation principles of the continuous problem on the discrete level is outlined. To solve the algebraic systems, **geometric multigrid (GMG) preconditioning** with **local Vanka-type smoother** of **GMRES** iterations is suggested. The performance of the STFEMs and GMG preconditioning technique is investigated numerically for challenging three-dimensional test problems [M. Anselmann, M. Bause, N. Margenberg, P. Shamko, An energy-efficient GMRES-Multigrid solver for space-time finite element computation of dynamic poro- and thermoelasticity, in progress].

Higher order convergence for the wave equation with rough coefficients

Krumbiegel, Felix *(Friedrich-Schiller-Universität Jena, Germany)*
Maier, Roland *(Friedrich-Schiller-Universität Jena, Germany)* 15:10

In this talk we will introduce a multiscale method for the wave equation with highly oscillatory and arbitrary rough coefficients, which achieves convergence rates beyond lowest order in space and time. We combine a high-order space discretization based on the Localized Orthogonal Decomposition method with a suitable implicit time stepping scheme. We further enhance the space discretization using so-called bubble functions to increase the stability of the method. The talk will focus on the techniques used to proof the higher order error estimate for the induced energy norm, and specifically on necessary stability conditions and the different error contributions. In the end we will give some numerical examples to show the convergence rates of the method.

Adaptive discretizations for temporal multiscale problems

Richter, Thomas *(Otto-von-Guericke Unviersität Magdeburg, Germany)*
Frei, Stefan *(Universität Konstanz)*
Leopold, Lautsch *(Otto-von-Guericke Unviersität Magdeburg, Germany)* 15:30

Many problems in science and engineering involve multiple scales in time. Examples are biological growth processes, e.g. growth of anorysm in pulsating blood fow or material fatigue of structures undergoing osciallations. In such systems, the interest often lies in the long-term dynamics, but not in the details of the fast processes. However, these are an essential part of the coupled dynamics and must therefore be represented correctly.

A resolved discretization of all scales is mostly not possible, e.g. if we model the aging of a structure over decades, which depends on forces on all scales, up to oscillations caused by, for instance, the wind.

We present a temporal multirate scheme that allows for the efficient simulation of long term processes by splitting the problem into an averaged long-term problem and localized fast scale problems. Plenty of discretization parameters must be chosen and we discuss means for an adaptive control of this complex algorithm based on a posteriori error estimators.

References

[1] S. Frei and T. Richter. Efficient approximation of flow problems with multiple scales in time. SIAM Multiscale Modeling and Simulation, 18(2):942–969, 2020. (https://doi.org/10.1137/19M1258396)

[2] L. Lautsch and T. Richter. Error estimation and adaptivity for differential equations with multiple scales in time. Computational Methods in Applied Mathemacics, 2021 (https://doi.org/10.1515/cmam-2021-0030)

An optimally stable discretization scheme for parametrized convection-dominated problems

Renelt, Lukas *(University of Münster, Germany)*
Engwer, Christian *(University of Münster, Germany)*
Ohlberger, Mario *(University of Münster, Germany)*

15:50

A known challenge in the numerical treatment of convection-dominated problems is the stability of the chosen discretization. One stable approach is the enrichment of the test space by supremizers leading to a nonsymmetric Petrov-Galerkin scheme. These supremizers are, however, expensive to compute as this requires the (approximate) solving of a partial differential equation for each trial basis function. In the context of model order reduction this also poses an additional challenge since both a reduced trial and test space need to be constructed simultaneously while preserving the stability in the reduced problem. We adapt the construction introduced by Brunken et al. for linear transport and recently also employed by Henning et al. for the wave equation. The main idea is choosing a test space first and then subsequently determining a corresponding trial space. This idea is computationally less difficult and leads to an optimally stable reduced scheme. However, the resulting "optimal trial spaces" are of a non-standard type and might even be parameter-dependent. We show that the approach allows for an easy construction of local reduced spaces which is particulary desirable in the case of spatially strongly varying data functions. First numerical experiments with parametrized convection-diffusion-reaction problems, as well as with convection-reaction systems show the advantages and challenges of the proposed approach. The analysis of the system reveals the saddle point structure of the underlying problem and thus gives a guideline for efficient solving.

S18-02: Numerical methods for differential equations

Date: May 31, 2023 08:30-09:30
Room: HSZ/H02

Higher-order semi-explicit time integration methods for poroelasticity problems

Altmann, Robert *(Universität Augsburg, Germany)* 08:30
Mujahid, Abdullah *(Universität Augsburg, Germany; Universität Stuttgart, Germany)*
Unger, Benjamin *(Universität Stuttgart, Germany)*

The linear Biot poroelasticity model with and without the quasi-static assumption give rise to coupled elliptic-parabolic and coupled hyperbolic-parabolic partial differential equations (PDEs), respectively. Semi-explicit time integration methods for these coupled PDEs enable decoupled solves with efficient solvers and black-box preconditioners for the subsystems. Hence, this reduces the computational burden that is associated with solving the coupled PDEs monolithically. The design of these specialized semi-explicit time integration methods is based on constructing well-posed PDEs containing time-delays, that naturally decouple the original PDE and approximate its solution up to a given order. An appropriate order implicit Runge-Kutta time discretization then yields the semi-explicit methods which are multi-step by construction.

In this talk, we will first discuss the key differences between well-posed delay systems that approximate the elliptic-parabolic PDEs and the hyperbolic-parabolic PDEs, respectively. This include the conditional stability of the delay systems or the restriction on the time-delay with respect to the parameters of the PDEs. Moreover, we present the ideas of the stability and the convergence analysis for higher-order semi-explicit methods and demonstrate the same with numerical examples.

Port-Hamiltonian descriptor systems and structure-preserving time integration

Morandin, Riccardo *(Technische Universität Berlin, Germany)* 08:50
Mehrmann, Volker *(Technische Universität Berlin, Germany)*

Port-Hamiltonian (pH) systems arising from the modeling of complex networks often present hidden algebraic constraints, representing for example the interconnection of different system components. This makes the treatment of differential-algebraic equations (DAEs), also known as descriptor systems, necessary. While for specific problem instances one can often reduce these systems to regular ODEs, it is useful to have general purpose discretization schemes that can be applied directly to DAEs, with the goal of preserving both the algebraic constraints and the pH structure of the problems. This is especially important in the case of automatized modelling.

In this talk we present a convenient and general formulation for port-Hamiltonian descriptor systems (pHDAEs). While this formulation is quite flexible and can be adapted for the application to infinite-dimensional systems, in this talk we primarily focus on the case of finite-dimensional DAEs. Furthermore, we briefly introduce several time integration schemes that

exploit the Dirac structure associated to the pH system, allowing the preservation of some of the system properties.

The talk is based on joint work with Volker Mehrmann.

Applications of numerical homotopy continuation for nonlinear boundary value problems

Anastasopoulos, Lysandros *(n.a.)* 09:10

Obtaining an equilibrium solution for a linear boundary value problem is a relatively simple process with proven analytical tools available. For nonlinear systems on the other hand, reaching a stationary solution can be more challenging and might necessitate a numerical approach, e.g. the Newton-Raphson method, which is initiated at a first estimate solution state. A related approach is the homotopy continuation technique. It differs from the classical Newton-Raphson method in that, first an auxiliary linear boundary value system is introduced, the equilibrium state of which can be calculated directly by matrix algebra, while afterwards the linear problem is gradually adjusted towards the nonlinear one, by a predictor-corrector algorithm. In this way, a numerical solution state of the original nonlinear problem can be reached.

Numerous physical processes in nature are governed by boundary value problems (BVP) describing a stationary system state, e.g. steady-state heat transfer, static deformation of structures and the electrostatic potential due to a charge density. Modelling such processes is often performed by time-independent partial differential equations, containing derivatives solely with respect to the spatial coordinates. These so-called boundary value problems constitute a special case of differential algebraic equations (DAE) in that they do not begin at a given state specified by initial conditions and progress with time, but instead have to be solved simultaneously on the entire domain while the time is fixed. Boundary conditions constrain the set of solutions, and are usually of Dirichlet type (value of function), or Neumann type (value of a partial derivative).

Numerical continuation is a concept utilized in algebraic equations or in dynamical systems with the goal to track the variation of a solution subject to variations of a parameter of interest. In the context of nonlinear boundary value problems, this parameter can be defined to vary between 0 and 1, where for the former value the system is linear, while for the latter value, the system is fully nonlinear. For progressing the solution along the arc from 0 to 1, the involved algorithms encompass a predictor-corrector scheme for, based on a direction determined by numerically calculated partial derivatives, as well as arc-length control and error norm monitoring. This work presents a practical application of the described method in one-dimensional heat transfer with finite difference discretization, where the thermal radiation introduces a nonlinearity term. Benefits and challenges of homotopy continuation in nonlinear boundary value problems are presented and evaluated.

S18-03: Numerical methods for differential equations

Date: May 31, 2023 14:00-16:00
Room: HSZ/H02

Structure-preserving numerical methods for dispersive wave equations

Ranocha, Hendrik *(Universität Hamburg, Germany)* 14:00

The numerical simulation of tsunami propagation is often based on the classical shallow water equations. However, there are several regimes where the assumptions used to derive this model are not satisfied. In this case, higher-order effects need to be taken into account, leading to nonlinear dispersive wave equations. Several variants of such models exist and are used in practice. In this contribution, we concentrate on the development and analysis of structure-preserving numerical methods. In particular, we will consider invariants such as the total energy and study efficient numerical methods yielding qualitative and quantitative improvements compared to standard schemes.

Advances on cut-cell stabilization methods for hyperbolic PDEs

Engwer, Christian *(WWU Münster, Germany)*
Birke, Gunnar *(WWU Münster, Germany)*
May, Sandra *(Uppsala University, Sweden)* 14:40

Cut-cell (or unfitted) methods have gained a lot of interest in the recent year. They are very attractive as they allow to weakly impose boundary and coupling conditions along interface not resolved by the finite element mesh. The underlying idea is to employ a simple structured mesh and incorporate the geometry by locally modifying the cell geometry, intersecting it with the domain geometry. A well known problem in this case is the fact that the codimension 0 intersection between an individual mesh cell and the physical domain might become arbitrarily small, which leads to numerical instabilities. In the last few years different stabilization techniques have been proposed to avoid these stability issues and, in particular, allow to use explicit time steps to solve hyperbolic conservation laws on cut-cell meshes; examples are the domain-of-dependence (DoD) stabilization proposed by the authors or the state-redistribution (SRD) method by A. Giuliani and M. J. Berger. In this talk will discuss recent advances of the DoD method and the relation to the SRD method.

On discrete ground states of rotating Bose–Einstein condensates

Yadav, Mahima *(Ruhr-University Bochum, Germany)*
Henning, Patrick *(Ruhr-University Bochum, Germany)* 15:00

The talk focuses on the study of ground states of Bose-Einstein condensates in a rotating frame. The ground states are described as the constrained minimizers of the Gross-Pitaevskii energy functional with an angular momentum term. The problem is discretized using Lagrange finite element spaces of arbitrary polynomial order and the approximation properties of the corresponding numerical approximations are presented, taking into account the missing uniqueness of ground states which is mainly caused by the invariance of the energy

functional under complex phase shifts. Error estimates of optimal order are shown for the L2- and H1-norm, as well as for the ground state energy and chemical potential.

A posteriori error analysis of the inf-sup constant for the divergence

Gallistl, Dietmar *(U Jena, Germany)* 15:20

Two a posteriori error estimates for a numerical approximation scheme for the inf-sup constant for the divergence (also known as the LBB constant) are shown. Under the assumption that the inf-sup constant is an eigenvalue of the Cosserat operator separated from the essential spectrum and that the mesh size is sufficiently small, the first estimate bounds the eigenvalue and eigenfunction errors from above and below by an error estimator up to multiplicative constants. In the second error estimate the reliability constant converges to 1 as the mesh size decreases, at the expense of a suboptimal efficiency estimate, and so allows for guaranteed enclosures of the inf-sup constant on sufficiently fine meshes.

A posteriori error estimates for H^2 nonconforming finite element methods on fourth order elliptic problems

Tian, Shudan *(Jena University, Germany)*
Gallistl, Dietmar *(Jena University, Germany)* 15:40

This talk will introduce a posterior error estimator for general H^2-nonconforming elements on the biharmonic equation and the fourth order perturbation problem in 2D and 3D. High order or C^0 but H^2-nonconforming elements usually with bubble functions, which can not be controlled by the weak continuity. By using projection technical, we prove the reliability. The efficiency are also presented in this article. The uniformly construction of a posterior error estimator can apply on most of H^2-nonconforming elements. The numerical experiments also confirm our construction.

S18-04: Numerical methods for differential equations

Date: June 1, 2023 16:00-19:00
Room: HSZ/H02

Discrete Helmholtz Decompositions

Bringmann, Philipp *(Humboldt-Universitaet zu Berlin)* 16:00
Ketteler, Jonas *(Universitaet Leipzig, Germany)*
Schedensack, Mira *(Universitaet Leipzig, Germany)*

Discrete Helmholtz decompositions have been proved in different contexts for piecewise constant vector fields. This talk generalizes those decompositions into piecewise gradients and rotations of discrete (finite element) functions to the 3d case and to piecewise affine vector fields. While the decomposition of piecewise constant vector fields consist of one conforming and one non-conforming part, the decomposition of piecewise affine vector fields require a nonconforming enrichement in both parts.

Finite element approximation for second order linear PDE in nondivergence form

Tran, Ngoc Tien *(Friedrich-Schiller-Universität Jena, Germany)* 16:40

This talk presents a novel technique for the approximation of strong solutions to uniformly elliptic linear PDE in nondivergence form with continuous leading coefficient in nonsmooth domains by finite element methods. These solutions satisfy the Alexandrov-Bakelman-Pucci (ABP) maximum principle, which provides an a posteriori error control for C1 conforming approximations. By minimizing this residual, we obtain an approximation to the exact solution in the maximum norm. Although discontinuous functions do not satisfy the ABP maximum principle, this approach extends to nonconforming FEM as well thanks to well-established enrichment operators. Convergence of the proposed FEM is established for uniform mesh-refinements. The built-in a posteriori error control (even for inexact solve) can be utilized in adaptive computations for the approximation of singular solutions, which performs superiorly in the numerical benchmarks in comparison to the uniform mesh-refining algorithm.

Implementation of equilibration-based a-posteriori error estimators into the FEniCSx finite element framework

Brodbeck, Maximilian *(University of Stuttgart, Germany)* 17:00
Bertrand, Fleurianne *(University of Twente, Netherlands)*
Ricken, Tim *(University of Stuttgart, Germany)*

Numerical solutions of, e.g., (poro-)elasticity or heat-conduction suffer from the deterioration of the overall accuracy when re-entrant corners, internal respectively boundary layers or shock-like fronts are present [1]. Estimates of the overall error, based on the numerical solution, offers a systematic way of retaining accuracy by localized mesh refinements. Following the seminal idea of Prager and Synge [2] for the Poisson equation, such error estimates can be constructed based on the comparison of fluxes, directly calculated from the approximation,

and any H(div) conforming function, satisfying the equilibrium condition. This function is typically called the reconstructed flux. More recently, this idea has been extended to linear-linear elasticity or the Biot equations [3,4]. Due to computational efficiency, the reconstructed flux is calculated locally. Focusing on conforming finite-element-discretisations, this requires - unlike, e.g., for error estimators of the Bank-Wiser type, where the error can be calculated in an element-wise manner - the solution of constrained minimization problems on local patches [5]. Within this contribution, we discuss efficient implementations of the equilibration procedure within the finite element framework FEniCSx. Testcases based on the Poisson equation and a comparison of this type of error estimator with a recently published implementation of a Bank-Weiser estimator [6] will be given.

[1] R. Verfürth. “A posteriori error estimation and adaptive mesh-refinement techniques”. In: J. Comput. Appl. Math 50 (1994).
[2] W. Prager and J. L. Synge. “Approximations in elasticity based on the concept of function space”. In: Quart. Appl. Math. 5 (1947), pp. 241-269.
[3] F. Bertrand, B. Kober, M. Moldenhauer, and G. Starke. “Weakly symmetric stress equilibration and a posteriori error estimation for linear elasticity”. In: Numer. Methods Partial Differ. Equ. 37 (2021).
[4] F. Bertrand and G. Starke. “A posteriori error estimates by weakly symmetric stress reconstruction for the Biot problem”. In: Comput. Math. with Appl. 91 (June 2021).
[5] D. Braess and J. Schöberl. “Equilibrated residual error estimator for edge elements”. In: Math. Comp. 77 (2008).
[6] R. Bulle, J. S. Hale, A. Lozinski, S. P. A. Bordas, and F. Chouly, “Hierarchical a posteriori error estimation of Bank-Weiser type in the FEniCS Project,” Comput. Math. with Appl. 131 (2023).

Dynamic boundary conditions and bulk-surface splitting methods

Altmann, Robert *(University of Augsburg, Germany)* 17:20
Zimmer, Christoph *(University of Augsburg, Germany)*

Dynamic boundary conditions enable the reflection of effective properties on the surface of the domain. For the numerical approximation of such (coupled) systems, we discuss several bulk-surface splitting schemes. Within this talk, we show first (respectively second)-order convergence for the parabolic case under the assumption of a weak CFL-type condition.

Least-Squares methods for coupled eigenvalue problems

Bertrand, Fleurianne *(University of Twente, The Netherlands)* 17:40

Determining the response of materials to a given phenomenon is crucial to our description of the world. In particular, recently discovered complex materials with unique features and usu- ally specific microstructure are key to much technology. The corresponding fundamental math- ematical problems are eigenvalue problems arising from coupled partial differential equations. In this talk, we discuss spectral properties of operators associated with the corresponding least- squares finite-element minimization of the residual. The convergence of the discrete eigenvalues and eigenfunctions towards the corresponding continuous eigenmodes is studied and analyzed with the help of appropriate L2 error estimates. A priori and a posteriori estimates are proved.

[1] Bertrand, Fleurianne, and Daniele Boffi. ”First order least-squares formulations for eigenvalue problems.” IMA Journal of Numerical Analysis 42.2 (2022): 1339-1363.
[2] Bertrand, Fleurianne, and Daniele Boffi. ”Least-squares formulations for eigenvalue problems associated with linear elasticity.” Computers & Mathematics with Applications 95 (2021): 19-27.

Constrained First-Order System Least Squares for Elastoplasticity

Starke, Gerhard *(Universität Duisburg-Essen, Germany)*
Schneider, Henrik *(Universität Duisburg-Essen, Germany)*
18:00

For the discretization of the variational inequalities modelling elastoplastic material behavior, a constrained first-order system least squares formulation is proposed and investigated in this paper. This approach simultaneously provides finite element approximations for displacements and stresses, in the Sobolev spaces H1 and H(div), respectively. Coercivity of the underlying bilinear form is proved under suitable assumptions on the hardening laws for a plastic flow rule of von Mises type. Our formulation is momentum-conservative in an elementwise fashion and does not degradate for (nearly) incompressible materials. This is even true if piecewise affine continuous functions (for the displacement components) are combined with lowest-order Raviart-Thomas elements (for the rows of the stress tensor). A semi-smooth Gauß-Newton method is set up based on the Newton derivative of the first-order system for the solution of the arising non-smooth nonlinear problems. Finally, computational results for common benchmark examples are shown including experiments for the limiting case of perfect plasticity.

[1] Adler. J.H., Vassilevski, P.S.: Error analysis for constrained first-order system least-squares finite-element methods. SIAM J. Sci. Comput. 36 (2014)
[2] Starke, G.: An adaptive least-squares mixed finite element method for elasto-plasticity. SIAM J. Numer. Anal. 45 (2007)

A central scheme for coupled systems of conservation laws

Kolbe, Niklas *(RWTH Aachen University, Germany)*
Herty, Michael *(RWTH Aachen University, Germany)*
Müller, Siegfried *(RWTH Aachen University, Germany)*
18:20

The coupling of PDE models at an interface has various applications, including two-phase dynamics and network models. We propose a new numerical approach for the coupling of systems of conservation laws, in which the solution of the original, possibly nonlinear, Riemann problem is not required. The approach is based on a relaxation limit taken at the interface and embedded in an asymptotic preserving finite volume method. It allows for a wide class of coupling conditions that we discuss in this talk, in particular, physically motivated coupling conditions for the original system can be suitably transformed. We present various numerical experiments for gas dynamics and fluid-structure coupling.

Numerical approximation of generalized solutions to the Ericksen–Leslie equations

Lasarzik, Robert *(Weierstrass Institute, Berlin, Germany)*
Reiter, Maximilian *(TU Berlin, Germany)*

18:40

We define the concept of energy-variational solutions for the Ericksen-Leslie equations in three spatial dimensions. This solution concept is finer than dissipative solutions and satisfies the weak-strong uniqueness property. For a certain choice of the regularity weight, we construct an energy-variational solution with the help of an implementable, structure-inheriting space-time discretization. The proposed scheme implements the main properties of the continuous system including the unit-norm restriction at every node of the mesh. Computational studies are performed in order to provide some evidence of the applicability of the proposed algorithm.

S18-05: Numerical methods for differential equations

Date: June 2, 2023 08:30-10:30
Room: HSZ/H02

Fast semi-iterative finite element Poisson solvers for Tensor Core GPUs

Ruda, Dustin *(TU Dortmund University, Germany)* 08:30
Turek, Stefan *(TU Dortmund University, Germany)*
Ribbrock, Dirk *(TU Dortmund University, Germany)*
Zajac, Peter *(TU Dortmund University, Germany)*

The overarching theme of the work presented is how specialized high performance hardware in the form of Tensor Core GPUs can be extensively exploited for PDE computing. For example, one representative of this hardware, the NVIDIA A100, promises a performance of up to 156 TFLOP/s in single precision and 312 TFLOP/s in half precision, but only if dense matrix operations are performed in the mentioned lower precision floating point formats which makes its use in the context of finite element simulations for ill-conditioned Poisson problems challenging. Novel direct and semi-iterative hardware-oriented finite element Poisson solvers that meet the requirements for exploiting the Tensor Cores are presented. These solvers incorporate explicit preconditioning, referred to as '*prehandling*' techniques, to reduce the condition number and thus ensure sufficient accuracy, using hierarchical bases in 2D or generating systems that have this property in the 3D case, respectively. By subsequently applying a Schur complement and exploiting the presence of similar mesh cells, the large, sparse linear system is transformed into multiplications of small, primarily dense matrices. The direct variant of the method has proven to be highly performant but is limited to special cases in terms of the mesh and finite element space and to the 2D case due to its storage requirements (see e.g. *Very fast finite element Poisson solvers on lower precision accelerator hardware: A proof of concept study for Nvidia Tesla V100* in The international Journal of High Performance Computing Applications 36(4), 2022). To extend the possible applications of this idea to higher order spaces, further differential operators and also the 3D case, we consider a semi-iterative variant. It consists mainly of a direct part, complemented by an iterative part given by the conjugate gradient method to solve a smaller part of the unknowns. The main focus is on the new results concerning prehandling in 3D and the algorithmics of the semi-iterative method, including estimates of storage requirements and complexity, as well as studies of its accuracy when using lower precision.

Adaptive mesh refinement in HPC and applications in the geosciences

Burstedde, Carsten *(Institute for Numerical Simulation, University of Bonn, Germany)* 08:50

Adaptive mesh refinement becomes a critical technique when a numerical simulation exhibits disparate scales and localized, possibly moving features. Refining the mesh only where needed, coarsening elsewhere, and repartitioning frequently can greatly improve the ratio of numerical error to numerical effort as well as the wall time to solution. Naturally, this approach requires a certain investment, namely to enhance the discretization and solver to accomodate adaptivity, and to execute mesh refinement with appropriate, fast and scalable

algorithms. While the first task may seem daunting at first, necessary modifications to the code are mostly local and well isolated. The second task is often too inolved to be addressed by a single simulation scientist, but can be delegated to freely available software libraries. Successfully adopting the conventions imposed by that software is, ideally, rewarded by inheriting its performance. In this talk, we discuss the algorithm design fundamental to the p4est software for scalable adaptive mesh management, and outline how to benefit from interfacing to it. p4est is being used in many projects, including geoscientific applications, and we close with selected examples.

Pendulum dynamics on a quantum computer with fixed-point arithmetic and the Runge-Kutta method

Mielke, André *(University of Stuttgart Germany, Germany)* 09:10
Ricken, Tim *(University of Stuttgart Germany, Germany)*

Quantum computers hint at significant speedup potential for numerical algorithms compared to their currently best known classical counterparts [1,2]. While there are no guarantees of superiority for quantum algorithms to generally outperform classical computers, with the exception of Grover's algorithm [3], quantum computing opens up a completely new way of thinking about problems and formulating solutions. Since ordinary differential equations are ubiquitous in science and engineering, finding faster or more accurate solution methods would benefit a wide variety of fields. Here, we use quantum solution methods from [4] to solve the differential equation describing a pendulum and analyze the drift behavior by comparing to classical solution schemes.

[1] Harrow, A.W.; Hassidim, A.; Lloyd, S.: Quantum algorithm for solving linear systems of equations.
[2] Peruzzo, A.; McClean, J.; Shadbolt, P.; Yung, M.; Zhou, X.; Love, P.J.; Aspuru-Guzik, A.; O'Brien, J.L.: A variational eigenvalue solver on a photonic quantum processor.
[3] Grover, L. K.: A fast quantum mechanical algorithm for database search.
[4] Zanger, B.; Mendl, C.B.; Schulz, M.; Schrieber, M.: Quantum Algorithms for Solving Ordinary Differential Equations via Classical Integration Methods.

The Bulk Trace FEM for the Simultaneous Solution of Structural Membranes on all Level-sets over a Bulk Domain

Fries, Thomas-Peter *(Institute of Structural Analysis, Graz University of Technology, Austria)* 09:30
Kaiser, Michael Wolfgang *(Institute of Structural Analysis, Graz University of Technology, Austria)*

We consider the simultaneous modelling and numerical simulation of partial differential equations on curved manifolds that are implied by all level-sets over some bulk domain. That is, the background domain together with some level-set function define the infinitely many domains of interest. Every level-set is an independent manifold with boundaries at the intersection with the boundary of the background domain. Our focus is on applications on curved surfaces in the three-dimensional space coming from structural mechanics such as membranes and shells [1]. For the numerical analysis, the background domain is discretized by higher-order elements which are by no means aligned with the level-sets. The resulting

method is a hybrid of the conforming Surface FEM and the non-conforming Trace FEM [2]. It simultaneously solves manifold applications on **all** level-sets of a level-set function in a background mesh (rather than only **one** level set as in the Trace FEM). A shared feature with the Surface FEM is that the background mesh provides the shape functions for the analysis and is used for the numerical integration of the weak form (without any cut elements nor need for stabilization). However, the fact that the domains of interest are implied as additional information and that the elements are not aligned or conforming to any of these manifolds are rather shared properties with fictitious domain methods in general and the Trace FEM in particular [3]. Boundary conditions for the individual level-set domains are easily prescribed through the background mesh. It seems natural to label the resulting approach, which herein is applied in the context of structural membranes and ropes in large displacement theory, the "Bulk Trace FEM". We note that mostly in the context of transport models, the Bulk Trace FEM is closely related to the methods discussed in [4].

[1] T.P. Fries, D. Schöllhammer: A unified finite strain theory for membranes and ropes, *Comp. Methods in Appl. Mech. Engrg.*, 113031, **365**, 2020.
[2] D. Schöllhammer, T.P. Fries: A Higher-order Trace Finite Element Method for Shells, *Internat. J. Numer. Methods Engrg.*, **122**, 1217-1238, 2021.
[3] M.A. Olshanskii, A. Reusken: Trace Finite Element Methods for PDEs on Surfaces, Lecture Notes in Computational Science and Engineering, **121**, Springer, Cham, 2017.
[4] G. Dziuk and C. M. Elliott, Finite element methods for surface PDEs, *Acta Numerica*, **22**, p. 289-396, 2013.

Solving Partial Differential Equations on (Evolving) Surfaces with Radial Basis Functions

Wendland, Holger *(University of Bayreuth, Germany)* 09:50

Radial basis functions (RBFs) provide flexible and powerful tools for the reconstruction of unknown functions from scattered samples or measurements. Their meshfree nature makes them a natural choice for solving a variety of problems on irregular domains, possibly in high-dimensional spaces or on manifolds.

The approximation space is usually formed using the shifts of a fixed basis function. This simple approach makes it easy to construct approximation spaces of arbitrary smoothness and in arbitrary dimensions. It is also possible to incorporate physical features like incompressibility into the approximation space.

In this talk, I will discuss how RBFs can be used to solve partial differential equations numerically on - possibly growing or evolving - surfaces. I will discuss error and stability estimates and give several examples.

Formation of wrinkles in a bi-layer system using manifold-valued finite elements

Nebel, Lisa Julia *(TU Dresden, Germany)*
Sander, Oliver *(TU Dresden, Germany)* 10:10

We model the formation of wrinkles of an elastic substrate coated with a thin film. The elastic substrate is first stretched, then the film is attached to a part of the substrate boundary in the deformed state. Once the external force is released, wrinkles form due to the stress mismatch

between the two materials. The elastic substrate is modeled using a hyperelastic, homogeneous and isotropic material. The film is modeled using a geometrically exact Cosserat shell. The resulting deformation and microrotation (φ,R) are a minimizing pair of the combined energy functional $J(\varphi,R) = \int_\Omega W_{bulk}(\nabla\varphi)\,dV + \int_{\Omega_c} W_{bulk}(\nabla\varphi_{|\Gamma_c},R)\,dS$ in a suitable Sobolev space. We discretize the problem using Lagrange finite elements for the substrate displacement. For the numerical treatment of the microrotation field, standard Lagrange finite elements cannot be used, as the microrotation field maps to the nonlinear manifold SO(3). We present a generalization of Lagrange finite elements that is suitable for such manifold-valued functions: geometric finite elements. We compare two ways of constructing them, one using an embedding of a nonlinear manifold into R^N and another using an intrinsic construction.

The resulting finite element spaces are complete and invariant under isometries of the manifold. The best approximation error depends on the mesh size h. We prove the existence of solutions of the discrete coupled model. Numerical experiments show that we can efficiently reproduce wrinkling patterns of coupled systems. Our approach works as well for more complex scenarios like multi-layer systems or systems involving various stress-free configurations.

S18-06: Numerical methods for differential equations

Date: June 2, 2023 11:00-13:00
Room: HSZ/H02

Adaptive unstructured T-splines for linear elasticity

Maier, Roland *(Friedrich Schiller University Jena, Germany)* 11:00
Morgenstern, Philipp *(Leibniz University Hannover, Germany)*
Takacs, Thomas *(Johann Radon Institute for Computational and Applied Mathematics of the Austrian Academy of Sciences, Linz, Austria)*

T-splines, actually a CAD technology, are one possible realization of B-splines on meshes with hanging nodes, where unstructured T-splines require additional strategies for the handling of extraordinary nodes, i.e. interior vertices of valency different from 4 and boundary vertices of valency greater than 3. In the context of Isogeometric analysis, they have been used as Ansatz functions for Galerkin schemes, beside other competing approaches to adaptive spline techniques such as Hierarchical splines, LR splines and many more. We present a local refinement scheme for T-splines of odd polynomial degree, that provides linear complexity, linearly independent spline bases, nested discrete spaces and uniformly bounded overlap of spline supports. We investigate its performance for simple model problems such as the Poisson problem and linear elasticity, accounting for conditioning of the system matrix and optimality of convergence rates.

A cost-efficient modified combined active-set Newton method for solving phase-field fracture into the monolithic limit

Kolditz, Leon Maximilian *(Leibniz Universität Hannover, Institut für Angewandte Mathematik, Germany)* 11:20
Mang, Katrin *(Leibniz Universität Hannover, Institut für Statik und Dynmaik, Germany)*
Wick, Thomas *(Leibniz Universität Hannover, Institut für Angewandte Mathematik, Germany; Université Paris-Saclay, LMPS - Laboratoire de Mecanique Paris-Saclay, France)*

In phase-field fracture simulation, a constraint variational inequality system, derived from the Francfort-Margio energy functional has to be solved. This problem is challenging due to two difficulties: Firstly, we have nonlinearities, which need to be treated. Secondly, it includes an inequality constraint that represents the irreversibility condition. The crucial nonlinearity can be resolved using an extrapolation depending on previous solutions to obtain a convex problem. The constraint can be treated with a primal-dual active set method. In a contribution from 2015, Timo Heister, Mary Wheeler and Thomas Wick introduced a concept for solving phase-field fracture problems with a primal-dual active set method and the concept of extrapolation, which were later included in the *pfm-cracks* code from 2020. Combined with a Newton method for solving the nonlinear phase-field fracture problem, we obtain a solution algorithm which seeks to minimize the Newton residual while achieving convergence in the active set at the same time. This implementation has two drawbacks: on the one hand, the extrapolation leads to time-lagging fracture growing phenomena. On the other hand, the active

set reveals slow convergence within the solution method. In this talk, we present an iteration on the extrapolation in order to iterate the problem to the monolithic limit. This neglects the time-lagging phenomena. Furthermore, three different suggestions for performance enhancements based on adjusting a constant, which takes a role during the computation of the active set. With a performance study, we substantiate the ideas by considering several quasi-static benchmarks in two or three dimensions.

High order biorthogonal basis functions

Beuchler, Sven *(LU Hannover, Germany)* 11:40

In this talk, we will present high order finite element discretizations using sparsity optimized basis functions. The aim of this contribution is to present biorthogonal functions to the above mentionted basis. We will discuss hexahedral and simplicial elements as well as situations on H^1, H(div) and H(Curl). This work is a collaboration with T. Haubold (Hannover) and J. Schoeberl (Vienna).

Algorithmic realization of exact three-point difference scheme for singular Sturm-Liouville problem

Khomenko, Nadiya *(Trier University, Germany; Pidstryhach IAPMM, National Academy of Sciences of Ukraine)*
Kutniv, Myroslav *(Pidstryhach IAPMM, National Academy of Sciences of Ukraine)*
Schulz, Volker *(Trier University, Germany)* 12:00

To approximate the Sturm-Liouville problem with difference schemes, there are usually used three-point difference schemes of the second order of accuracy. In previous works of the authors, for the Sturm-Liouville problem was developed an algorithmic realization of the exact three-point difference scheme through three-point difference schemes of high order of accuracy. We showed that the coefficients of the exact three-point difference scheme at any grid node can be expressed through the solutions of four auxiliary Cauchy problems, each of which can be solved approximately in one step by any one-step method. For the singular Sturm-Liouville problem exact and three-point difference schemes of high order of accuracy were proposed in [1]. However, in general case, coefficients of these difference schemes are expressed in terms of multiple integrals of coefficients of the differential equation at each node of the grid, which leads to difficulties in practical realization of such schemes. In our research we develop a new algorithmic realization of exact three-point difference schemes for the Sturm-Liouville problem with singular differential operator. We show that coefficients of the exact three-point difference scheme for singular Sturm-Liouville problem can be expressed via the solutions of auxiliary Cauchy problems.

[1] V. L. Makarov, I. P. Gavrilyuk, V. M. Luzhnykh “Exact and truncated difference schemes for one class of Sturm-Liouville problems with degeneration”, Differents. Uravn., 16, No. 7, 1265-1275, 1980.

Step size control for the Newton iteration for the p-Stokes equations decreases computation time

Schmidt, Niko *(Christian-Albrecht University of Kiel, Germany)* 12:20

The p-Stokes equations are nonlinear partial differential equations. Finding a solution of these equations is computationally expensive. Thus, Newton's method is often used to solve this problem with a small number of iterations. Newton's method is not globally convergent. Hence, we need a step size control. For the step size control, we need a minimization problem. The intuitive idea of using the residual norm for the minimization problem is computationally expensive. Instead, we use a convex functional, which is just an integral. Evaluating it has nearly no computational costs compared to calculating a direction with Newton's method. The convex functional is the anti-derivative of the variational formulation of the p-Stokes equations. This anti-derivative exists in divergence-free spaces. If we add a small diffusion term to the variational formulation of the p-Stokes equations, we can prove global q-superlinear convergence for Newton's method with Armijo step sizes. We compare this method with approximations of exact step sizes and the Picard iteration in an experiment.

Mixed FEM for Gradient Elasticity and the Singularly Perturbed Biharmonic problem

Ketteler, Jonas *(Univeristät Leipzig, Germany)*
Schedensack, Mira *(Univeristät Leipzig, Germany)*
Balzani, Daniel *(Ruhruniversität, Bochum)*
Riesselmann, Johannes *(Ruhruniversität, Bochum)* 12:40

The Gradient Elasticity problem consists of the Elasticity problem and a Bilaplace smoothing term scaled by a small parameter. The Smoothing term enforces that the second derivative of the solution is square integrable and therefore continuous. Therefore the solution does not have singularities in reentrant corners.

Since a conforming discretization of the Gradient elasticity problem is impractical to implement we split the problem into two Poisson problems and a general Stokes problem. We proof that the original problem and the splitted problem have unique solutions that coincide.

In our discretization of the splitted problem we only use standard Finite Element spaces which are easy to implement. For the discretization of the Poisson problems we use standard linear Lagrange elements.

For the discretization of the general Stokes problem we use standard linear Lagrange elements with stabilizing face bubbles and piecewise constant finite element functions for a first Lagrange parameter and linear Lagrange elements for a second Lagrange parameter. We proof uniqueness and existence of a discrete solution with quasi-best approximaiton properties. The main ingredient of the proof of the critical discrete inf-sup condition is a discrete Helmholtz decomposition.

Some numerical examples are shown.

We focus on the three dimensional problem. The two-dimensional problem can be treated analogously.

S18-07: Numerical methods for differential equations

Date: June 2, 2023 16:00-18:00
Room: HSZ/H02

Raviart-Thomas enriched Scott-Vogelius finite element methods for the Navier-Stokes equations

John, Volker *(Weierstrass Institute for Applied Analysis and Stochastics, Germany)*
Li, Xu *(Shandong University, China)*
Merdon, Christian *(Weierstrass Institute for Applied Analysis and Stochastics, Germany)*

16:00

This talk concerns discretizations for the incompressible Navier-Stokes problem, for which structural properties like the continuity requirement, the inf-sup stability and the divergence constraint are challenging to obtain simultaneously. Traditional finite element methods do not satisfy the divergence constraint exactly with the exception of Scott-Vogelius finite element methods, which are in general only stable on special meshes such as barycentrically refined meshes. The talk discusses a new approach which stabilizes the Scott-Vogelius elements on arbitrary shape-regular meshes by enriching the velocity space with some specially chosen Raviart-Thomas functions, such that the divergence-free property is maintained. This yields a discrete velocity solution that consists of an H1-conforming pressure-robust part and a small Hdiv-conforming part that can be added to obtain a divergence-free velocity field. Starting with the Stokes equations, inf-sup stability, error estimates, and in particular the pressure-robustness property of the newly proposed element is shown. Also a reduced version of the method with less numerical costs, equivalent to a P_k-P_0 discretisation, is presented. In the final part the new approach is extended to the Navier-Stokes problem, where also the convection-robustness property is of importance and suitable discretizations of the nonlinear term are discussed. Numerical examples validate all features.

On the design of global-in-time Navier-Stokes solvers

Lohmann, Christoph *(TU Dortmund University, Germany)*
Turek, Stefan *(TU Dortmund University, Germany)*

16:20

The work to be presented in this talk focuses on the design of a new global-in-time multigrid solution strategy for incompressible flow problems, which highly exploits the Pressure Schur complement (PSC) approach [2] and provides the possibility to use massively parallelizable solution components. For linear problems like the incompressible Stokes equations discretized in space using an inf-sup-stable finite element pair, the fundamental idea is to block the individual linear systems of equations at each time step into a single all-at-once saddle point problem for all velocity and pressure unknowns. Then the Pressure Schur complement can be used to eliminate the velocity fields and set up a linear system for all pressure variables only. This algebraic manipulation allows the construction of parallel-in-time preconditioners for the corresponding all-at-once Picard iteration by extending frequently used sequential PSC preconditioners in a straightforward manner (cf. [1]). We show that those preconditioners can be applied very efficiently on modern high performance computing facilities and are asymptotically exact in the limit of vanishing time increments.

To accelerate the convergence of the proposed fixed-point iteration, this iterative solver is embedded as a smoother into a space-time multigrid algorithm, where the computational complexity of the coarse grid problem highly depends on the coarsening strategy in space and/or time. Although coarsening in space using commonly used FE intergrid transfer operators is possible, most promising results could be obtained by only coarsening in time using tailor-made prolongation and restriction operators. This procedure even allows the efficient solution of the nonlinear Navier-Stokes equations for many time steps by employing Newton's method for linearization.

At the end, the presented multigrid solution strategy only requires the solution of time-dependent linear convection-diffusion-reaction equations and many Poisson problems, which both can be performed efficiently by using algorithms that exploit massive parallelism. The potential of this approach for CFD simulations with large time horizons on modern HPC architectures including accelerator hardware is illustrated in numerical examples.

[1] F. Danieli, B. S. Southworth, and A. J. Wathen, *Space-Time Block Preconditioning for Incompressible Flow*. SIAM Journal on Scientific Computing, 44.1, 2022.
[2] St. Turek, *On discrete projection methods for the incompressible Navier-Stokes equations: an algorithmical approach*. Computer Methods in Applied Mechanics and Engineering, Vol. 143.3, pp. 271-288, 1997.

Higher order discontinuous Galerkin methods in time and pressure-robust finite element discretizations applied to time-dependent Stokes problems

Ahmed, Naveed *(Gulf University for Science and Technology, Kuwait)*
Becher, Simon *(Technische Universität Dresden, Germany)*
Matthies, Gunar *(Technische Universität Dresden, Germany)*

16:40

We analyze finite element discretizations of the time-dependent Stokes equations that are based on discontinuous Galerkin time stepping schemes in combination with pressure-robust inf-sup stable finite element methods in space. The pressure-robustness enables error estimates for the velocity that are completely independent of the pressure. We prove optimal convergence orders in space and time for both velocity and pressure. Moreover, a cheap postprocessing allows to improve the temporal accuracy of the velocity, again with error constants independent of the pressure. Numerical examples illustrate our theoretical findings.

Immersed boundary method for the 3D compressible Navier-Stokes equation

Kristoffersen, Frederik *(Norwegian University of Science and Technology, Norway)*
Larsson, Martin *(Sportradar AS)*
Johnsen, Sverre Gullikstad *(SINTEF Industry)*
Schröder, Wolfgang *(North Rhine-Westphalia Technical University of Aachen)*
Müller, Bernhard *(Norwegian University of Science and Technology, Norway)*

17:00

Our research is motivated by the objective of simulating flow in the upper airways of obstructive sleep apnea (OSA) patients. OSA is a sleep related breathing disorder. Surgical treatments may cure OSA patients. However, it has proven difficult to predict the outcome of such surgeries, and in some cases they make the conditions even worse. Numerical simulation could

play a key role in predicting the outcome of an OSA surgery and whether a patient would benefit from it.

A numerical method to simulate air flow in complex geometries is developed. The future ambition for this method is its application to simulate respiratory flow in the upper airways of patients with OSA. This multiphysics phenomenon is challenging for several reasons. The geometry of the upper airways is complex and consists of highly different scales. Also, the surrounding tissue is not rigid or uniform, but will interact in different ways with the flow. Additionally, the tissue is subject to neural activity, which can move and change the mechanical properties of the flow boundaries.

The 3D sharp interface ghost-node-based immersed boundary method is a solid foundation for tackling this challenge. Near the sharp interface, the flow variables are reconstructed in the direction normal to the immersed boundary. The reconstruction is done using trilinear interpolation. By employing second order central finite differences for both convective and diffusive terms, the method will handle both concave and convex regions. The modelling equations are the 3D Navier-Stokes equations for compressible flow. With the compressible flow approach, it is also possible to study acoustic and thermal effects. For the time discretization, the classical explicit fourth order Runge-Kutta method is used.

The immersed boundary method for the 3D compressible Navier-Stokes equations is currently being verified and validated. It has shown good coherence with the literature for generic problems such as the cylinder cross flow test. It will be verified and validated by additional benchmark cases in the near future, before simulating flow in complex geometries such as the human upper airways.

Time-spectral extension to a compressible Navier-Stokes method with nested solution algorithms

Gros, Erik *(DLR-Institute of Software Methods for Product Virtualization)* 17:20
Haupt, Raphael *(DLR-Institute of Software Methods for Product Virtualization)*
Stueck, Arthur *(DLR-Institute of Software Methods for Product Virtualization)*

The Time Spectral Method (TSM) has a huge efficiency potential for the prediction of aerodynamic flows dominated by periodic influences such as rotor, propeller or oscillating wing analyses. Unlike well-established implicit time-stepping approaches in CFD, in which (one or several, usually non-linear) equation systems are solved per physical time step, the TSM leads to one large, nonlinear block-equation system. It couples the spectral coefficient fields at the collocation points in time that support the spectral ansatz. The spectral coefficients can be considered as discrete CFD solution fields at the collocation points referred to as time instances. We aim for a flexible implementation that enables strong implicit, solution hierarchies to benefit from the tailored ansatz in time. Unlike other time-discretization methods based on a spectral approach such as the Harmonic Balance technique, the TSM leads to real-valued equation systems and facilitates the implementation and integration in the framework of existing implicit CFD solvers. It allows to re-use huge portions of the underlying software infrastructure. The TSM method, the key features of which will be described in the offered talk/paper, was implemented in the CFD software CODA being developed as part of a collaboration between the French Aerospace Lab ONERA, the German Aerospace Center (DLR), Airbus, and their European research partners.

The numerical solution of coupled TSM equation systems tends to become more challenging with a growing number of time instances in the truncated spectral ansatz when a larger harmonic content is to be resolved. This is addressed by a nested solution strategy in this study: all time instances per finite element (or finite control volume) of the unstructured spatial mesh are block-inverted by means of an element-wise LU decomposition embedded in a block-Jacobi/Gauss-Seidel method, which - in turn - is used as a preconditioner to a Newton-Krylov (GMRES) scheme with implicit pseudo-time relaxation. Exact derivatives computed by algorithmic differentiation are available to drive the relaxed Newton-Krylov method. The influence of different realizations of solution hierarchies and choices of solution parameters involved will be discussed in the offered talk/paper for moving airfoil cases including compressible Reynolds-averaged Navier-Stokes computations with the one-equation Spalart-Allmaras turbulence model.

A structure-preserving ALE method for the two-phase Navier-Stokes flow

Garcke, Harald *(University of Regensburg, Germany)* 17:40
Nurnberg, Robert *(University of Trento, Italy)*
Zhao, Quan *(University of Regensburg, Germany)*

We consider the numerical approximation of a sharp-interface model for the two-phase Navier-Stokes flow, and propose a structure-preserving finite element method for the model, meaning that volume preservation and energy decay are satisfied on the discrete level. The constructed method is based on suitable discretizations of a novel arbitrary Lagrangian-Eulerian weak formulation. We prove the structure-preserving properties and present numerical examples to illustrate the robustness of the introduced method.

S19: Optimisation of differential equations

Organizer(s): **Geiersbach, Caroline** *(WIAS Berlin)*
Weiß, Olga *(U Hamburg)*

S19-01: Optimisation of differential equations

Date: May 30, 2023 13:30-16:10
Room: HSZ/101

Fully-corrective generalized conditional gradient methods for nonsmooth optimization

Walter, Daniel *(Humboldt Universität zu Berlin, Germany)* 13:30

Nonsmooth regularizers have become a cornerstone of modern inverse problem and optimal control theory. This is attributed to the observation that a suitable choice of the penalty function brings forth desired structural features in the solution of the associated minimization problems. However, this comes at the price of solving a nonsmooth minimization problem in which the underlying variable space lacks "nice" properties, such as reflexivity or uniform convexity. We propose *a fully-corrective generalized conditional gradient method* (FC-GCG) for the minimization of the sum of a smooth, convex loss function and a convex one-homogeneous regularizer over a Banach space. The algorithm relies on the mutual update of a finite set A_k of extremal points of the unit ball of the regularizer and of an iterate $u_k \in \text{cone}(A_k)$. Each iteration requires the solution of one linear problem to update A_k and of one finite dimensional convex minimization problem to update the iterate. Under standard hypotheses on the minimization problem we show that the algorithm converges sublinearly to a solution. Subsequently, imposing additional assumptions on the associated dual variables, this is improved to a linear rate of convergence. The proof of both results relies on two key observations: First, we prove the equivalence of the considered problem to the minimization of a lifted functional over a particular space of Radon measures using Choquet's theorem. Second, the FC-GCG algorithm is connected to a *Primal-Dual-Active-point Method* (PDAP) on the lifted problem for which we finally derive the desired convergence rates.

A topological derivative-based algorithm to solve optimal control problems with $L^0(\Omega)$ control cost

Wachsmuth, Daniel *(University of Wuerzburg, Germany)* 14:10

In this paper, we consider optimization problems with L^0-cost of the controls. Here, we take the support of the control as independent optimization variable. Topological derivatives of the corresponding value function with respect to variations of the support are derived. These topological derivatives are used in a novel algorithm. In the algorithm, topology changes happen at large values of the topological derivative. Convergence results are given.

On Integer Optimal Control Problems with Total Variation Regularization

Marko, Jonas *(BTU Cottbus-Senftenberg, Germany)*
Wachsmuth, Gerd *(BTU Cottbus-Senftenberg, Germany)* 14:30

We investigate integer optimal control problems where the goal is to minimize the objective $F(u) + \beta \mathrm{TV}(u)$ with $\beta > 0$ such that $u(t)$ is an integer for a.a. t. Here, TV(u) denotes the total variation of u, which penalizes jumps of the control.

The contribution F is assumed to be differentiable, e.g. it could realize the tracking of the state given by an ODE or PDE dependent on u. The presence of the TV-term can be used to prove the existence of a minimizer. Moreover, it averts rapid switching between multiple control levels in a short amount of time, which is desirable from an application point of view. Thus, optimization problems of this structure have an abundance of applications, as for example in multi-material topology optimization, in gas network control problems or in the placement of actuators and sensors for distributed parameter systems.

We show local optimality conditions of first and second order via a finite-dimensional switching point problem. Additionally, a non-local optimality condition treating back-and-forth switches will be formulated.
For a numerical solution, we propose a proximal gradient method. The emerging discretized subproblems will be solved by an algorithm which is polynomial in the mesh size and in the admissible control levels. An adaption of this algorithm can be used to handle subproblems of the trust-region method proposed in the work of Sven Leyffer and Paul Manns (see Reference 1). We show properties of the proximal gradient method and of the generated sequence of iterates. Finally, we showcase numerical results exemplary on two control problems, one governed by the Lotka-Volterra equations.

For further information, see Reference 2.

References:

1. Sven Leyffer, Paul Manns (2021). *Sequential Linear Integer Programming for Integer Optimal Control with Total Variation Regularization.* https://arxiv.org/abs/2106.13453.
2. J. Marko and G. Wachsmuth (2022). *Integer optimal control problems with total variation regularization: Optimality conditions and fast solution of subproblems.* https://arxiv.org/abs/2207.05503.

A semismooth* Newton method for contact problems with Coulomb friction

Mandlmayr, Michael *(OEAW, Austria)* 14:50

The semismooth* Newton method is a recent approach to tackle generalized equations. Semismooth* Newton methods can be viewed as a generalization of the classical Newton method, which additionally covers both the nonsmooth as well as the set-valued case. There are two main differences to classical approaches, [1] The linearization is done via the normal-cone of the graph (coderivative). [2] We need to perform an additional step that provides a point on the graph (Approximation step). We will introduce the basic ideas of this method and precent its application to contact problems with Coulomb friction. Moreover, we will precent results on the local order of convergence and show numerical experiments that are in line with these results.

Greedy algorithms for the reconstruction of operators in dynamical systems

Buchwald, Simon *(Universität Konstanz, Germany)* 15:10
Ciaramella, Gabriele *(MOX, Dipartimento di Matematica, Politecnico di Milano, Italy)*
Salomon, Julien *(INRIA Paris, France)*

We present a novel convergence analysis for greedy reconstruction algorithms based on the strategy presented in [Y. Maday and J. Salomon, Proceedings of the 48th IEEE Conference on Decision and Control, 2009, pp. 375-379]. These procedures allow the design of a sequence of control functions that ease the identification of unknown operators in dynamical systems. The original strategy of greedy reconstruction algorithms is based on an offline/online decomposition of the reconstruction process and on an ansatz for the unknown operator obtained by an a priori chosen set of linearly independent matrices. The presented convergence analysis focuses on the example of linear-quadratic (optimization) problems governed by linear dynamical systems and reveals a strong dependence of the performance of the greedy algorithm on the observability properties of the system and on the ansatz of the basis elements. Moreover, the analysis allows us to introduce a more robust optimized greedy reconstruction algorithm. This optimized approach also applies to nonlinear reconstruction problems, and its efficiency is demonstrated by numerical experiments.

High-accuracy numerical optimal control of dynamical systems with switches and state jumps

Nurkanovic, Armin *(University of Freiburg, Germany,)* 15:30
Diehl, Moritz *(University of Freiburg, Germany,)*

We present the method of the Finite Elements with Switch Detection (FESD), which is a high-accuracy numerical discretization method for ODEs with a discontinuous right-hand side. We regard the Filippov convexification of these systems and their transformations into dynamic complementarity systems. FESD is based on solving of nonlinear complementarity problems and able to automatically detect the switching events in time. If standard time-stepping Runge-Kutta (RK) methods are naively applied to a nonsmooth ODE, the accuracy is at best of order one and the numerical sensitivities are always wrong. In FESD, we let the integrator step-size to be a degree of freedom. Additional complementarity conditions, that we call cross complementarities, enable exact switch detection, hence FESD is able to recover the high-order accuracy, which the RK methods enjoy for smooth ODEs. Additional conditions called step equilibration allow the step-size to change only when switches occur and thus avoid spurious degrees of freedom. Convergence results for the FESD method are presented, local uniqueness of the solution and convergence of numerical sensitivities are proven. Our main application of FESD is within direct optimal control, i.e., a first-discretize-then-optimize approach. The efficacy of FESD in demonstrated on several simulation and optimal control examples. In an optimal control problem benchmark with FESD we achieve up to five orders of magnitude more accurate solutions than a standard approach for the same computational time.

Moreover, we outline the main ideas behind the time-freezing reformulation. It enables one to transform dynamical systems with state jumps (discontinuity in the state) into ODEs with a discontinuous right-hand side (discontinuity now only in the vector field). The main idea of

time-freezing is to introduce a clock state and an auxiliary dynamical system whose trajectory endpoints satisfy the state jump law. When the auxiliary system is active, the clock state is not evolving, hence by taking only the parts of the trajectory when the clock state was active, we can recover the original solution. For numerically solving optimal control problems subject to dynamical systems with state jumps, we can use the time-freezing reformulation (which is exact) and apply afterward the aforementioned FESD method. This enables the treatment of a broad class of nonsmooth systems in numerical optimal control in a unified way. All methods and examples we present are implemented in our open-source tool nosnoc (`https://github.com/nurkanovic/nosnoc`).

S19-02: Optimisation of differential equations

Date: May 31, 2023 08:30-09:30
Room: HSZ/101

Pressure-robustness in the context of optimal control of incompressible flows

Merdon, Christian *(WIAS, Germany)* 08:30
Wollner, Winnifried *(Universität Hamburg, Germany)*

The talk discusses the benefits of pressure-robust discretizations in the scope of optimal control of incompressible flows. Here, gradient forces appearing in the data can have a negative impact on the accuracy of state and control and can only be correctly balanced if their L^2 -orthogonality onto discretely divergence-free test functions is restored. Perfectly orthogonal divergence-free discretizations or divergence-free reconstructions of these test functions do the trick and lead to much better analytic a priori estimates that are also validated in numerical examples.

Space-time phase-field fracture as a constrained nonlinear optimization problem

Khimin, Denis *(Leibniz Universität Hannover, Germany)* 08:50
Steinbach, Marc C. *(Leibniz Universität Hannover, Germany)*
Wick, Thomas *(Leibniz Universität Hannover, Germany, Université Paris-Saclay, ENS Paris-Saclay, France)*

In this work we consider a space-time continuous phase-field fracture model as an abstract energy minimization problem in a Banach space. Within the derivation of the optimality conditions special emphasis is on the concrete choice of the function spaces and the required regularity. Afterwards we present a higher level optimal control problem, where the constraits are given by the previously derived optimality conditions of the lower level phase-field fracture.

Application of the SQP Method to Phase-Field Fracture Optimal Control Problems

Hehl, Andreas *(Rheinische Friedrich-Wilhelms-Universität Bonn, Germany)* 09:10
Neitzel, Ira *(Rheinische Friedrich-Wilhelms-Universität Bonn, Germany)*

We apply the sequential quadratic programming (SQP) method to a model problem with a simplified coupled quasi-linear partial differential equation, that stems from a regularized phase-field energy minimization problem. Using a phase-field approximation, an irreversibility condition on the fracture growth is handled by means of a penalization of the phase-field variable. We conduct numerical experiments to verify convergence rates that have been proven analytically for a related fracture propagation optimal control problem from [1].

[1] A. Hehl and I. Neitzel, *Local quadratic convergence of the SQP method for an optimal control problem governed by a reguralized fracture propagation model,* In Preparation, 2023.

S19-03: Optimisation of differential equations

Date: June 1, 2023 08:30-10:30
Room: HSZ/101

One-shot Learning of Surrogates in PDE-constrained Optimization Under Uncertainty

Guth, Philipp *(RICAM)* 08:30
Schillings, Claudia *(Free University Berlin)*
Weissmann, Simon *(University of Mannheim)*

Approaches to decision making and learning mainly rely on optimization techniques to achieve "best" values for parameters and decision variables. In most practical settings, however, the optimization takes place in the presence of uncertainty about model correctness, data relevance, and numerous other factors that influence the resulting solutions. For complex processes modeled by nonlinear ordinary and partial differential equations, the incorporation of these uncertainties typically results in high or even infinite dimensional problems in terms of the uncertain parameters as well as the optimization variables, which in many cases are not solvable with current state of the art methods. One promising potential remedy to this issue lies in the approximation of the forward problems using novel techniques arising in uncertainty quantification and machine learning. We propose in this talk a general framework for machine learning based optimization under uncertainty and inverse problems. Our approach replaces the complex forward model by a surrogate, e.g. a neural network, which is learned simultaneously in a one-shot sense when estimating the unknown parameters from data or solving the optimal control problem. By establishing a link to the Bayesian approach, an algorithmic framework is developed which ensures the feasibility of the parameter estimate / control w.r. to the forward model.

Deep Learning from an optimal control point of view with adaptive time stepping

Antil, Harbir *(George Mason University, U.S.A.)* 09:10
Diaz, Hugo *(University of Delaware, U.S.A.)*
Herberg, Evelyn *(University Heidelberg, Germany)*

We highlight the common features of optimal control problems with partial differential equations and deep learning problems. Furthermore, we introduce a new variable in the neural network architecture, which can be interpreted as a time step-size. The proposed framework can be applied to any of the existing networks such as ResNet or Fractional-DNN. This framework is shown to help overcome the vanishing and exploding gradient issues. The proposed approach is applied to an ill-posed 3D-Maxwell's equation.

Controlling the Vlasov-Poisson model using a Monte Carlo framework

Bartsch, Jan *(University of Konstanz, Germany)*
Knopf, Patrik *(University of Regensburg, Germany)*
Scheurer, Stefania *(University of Stuttgart, Germany)*
Weber, Jörg *(Lund University, Sweden)*

09:30

The Vlasov-Poisson equation describes the evolution of plasma in the so-called collisionless regime. The investigation of a high-temperature plasma that is influenced by an exterior magnetic field is one of the most significant aspects of the research on thermonuclear fusion. However, there are only a few works on optimal control problems governed by the Vlasov-Poisson. We formulate and analyse a Vlasov-Poisson kinetic optimal control problem where the control is assumed to be the external magnetic field. The purpose of this control is to drive an ensemble of particles to acquire a desired mean and variance in phase space. To characterize the optimal control, we use the widely known Lagrange multiplier framework to derive an optimality system. We build a Monte Carlo framework to solve all arising equations numerically and apply the Stochastic Approximation Average principle to solve the optimal control problem. We perform numerical experiments that successfully validate our optimization framework.

Stochastic Optimal Control of District Heating Networks under Demand Uncertainty

Heidrich, Johanna *(Fraunhofer-Institut für Techno- und Wirtschaftsmathematik ITWM, Germany)*

09:50

Operators of district heating networks are facing numerous technical challenges in course of the energy system transformation, which require innovations in network control. A realistic mapping of the energy transport through the distribution network is key to optimizing the use of operating resources. The underlying thermo-hydraulic PDE system strongly depends on the demand resulting from the heat consumers' behavior as a boundary condition, and consequently the demand has a considerable impact on optimization problems constrained by this PDE system as well.

As most district heating networks are equipped with little sensor technology, real-time monitoring data from heat consumers is rarely available to calibrate the simulation, and regardless of the data situation, for predictive optimization a demand forecasting needs to be provided. For these reasons, a realistic time-resolved demand prognosis has to be derived from the limited historical data available.

First, underlying patterns need to be identified. Using regression analysis of historical real monitoring data of different building types over the course of different seasons, we generate temperature-dependent, time-resolved, characteristic demand profiles of heat consumers.Next, we aim to incorporate the inherent stochastic nature of demand into our previous results. As underlying patterns can be recognized and demand only takes values in a bounded interval, we find the Jacobi process to be a stochastic process that captures these characteristics. We focus on Jacobi processes with time-dependent mean reversion levels, namely the demand profiles obtained above, and provide parameter fittings for different

building types. By applying the strategy presented here, a realistic time-resolved demand can be simulated only based on characteristic consumer variables.

Taking the consumers' inherently random behavior as solutions to stochastic differential equations into account, we intend to investigate its impact on the optimization results. The optimal control problem under consideration is to find the optimal input into the system such that not only the variables considered before are minimized but in addition the stochastic demands are satisfied. Propagating the uncertainty in its boundary condition through the PDE then results in a random field PDE solution and thus the objective function becomes a random variable, on which different risk measures could be applied for risk-neutral or risk-averse optimization. Solving such stochastic optimal control problems is not trivial, therefore we employ different strategies, e.g. a space mapping approach, and compare them regarding performance, computing time and robustness for our application example of a district heating network.

A novel homotopy approach based on exponentially modified Gaussian functions for the reliable determination of model parameters for chromatographic processes

Cebulla, Dominik H. *(TU Braunschweig, Germany)* 10:10
Kirches, Christian *(TU Braunschweig, Germany)*
Potschka, Andreas *(Clausthal University of Technology, Germany)*

Column liquid chromatography plays an important role in the downstream processing of biopharmaceuticals, where the goal is to capture and purify a target protein from a given mixture. We investigate a real-world ion exchange chromatography process, where a target protein must be separated from a single impurity. To mathematically describe this process we use the well-known transport-dispersive model in combination with the highly nonlinear steric mass action isotherm model. In our talk we particularly focus on the model calibration step, where we use a structure-exploiting variant of the generalized Gauss-Newton method to efficiently solve the resulting nonlinear least squares problems constrained by partial differential equations. However, multiple difficulties arise in this context. For example, some model parameters are completely unknown, hence the provided initial parameter guess may be far away from a solution. Furthermore, the crucial adsorption process cannot be directly measured. These and more difficulties often lead to a breakdown of the employed optimization method for parameter estimation. To overcome this undesired behavior, we present and investigate a novel homotopy approach based on exponentially modified Gaussian functions, the latter being known to describe chromatography data well. We will see that the proposed approach is capable of reliably determining suitable model parameters for given measurement data, even when starting far away from a solution. We conclude our talk with an outlook on the predictability of the calibrated model by comparing real-world data from the optimized chromatographic process with the prediction given by our model. We will see that the prediction and real-world behavior agree well and that the batch-cycle time of the optimized process could be reduced significantly.

S19-04: Optimisation of differential equations

Date: June 1, 2023 16:00-19:00
Room: HSZ/101

Optimization on Hilbert Manifolds

Schiela, Anton *(Universität Bayreuth, Germany)* 16:00

Usually, numerical algorithms solve problems, posed on linear spaces. However, there are a couple of instances, where the the domain of the problem is a non-linear manifold. In this talk we will give an overview of ideas, how to treat problems in this class numerically. This comprises gradient type methods, as well as Newton-type methods for unconstrained, but also for constrained optimization. As an example, we will consider an optimal control problem, subject to a state equation, that is posed on a non-linear Hilbert manifold.

Topology optimization of a bipolar plate

Baeck, Leon Niklas *(Fraunhofer Institute for Industrial Mathematics ITWM, Germany)*
Blauth, Sebastian *(Fraunhofer Institute for Industrial Mathematics ITWM, Germany)*
Pinnau, René *(RPTU Kaiserslautern-Landau, Germany)*
Sturm, Kevin *(TU Vienna, Austria)* 16:20

Hydrogen technologies are set to play a major role in the process of achieving climate-neutral mobility and a clean energy industry. In this context, the production of hydrogen with electrolysis cells is of high importance. Here, water is split into hydrogen and oxygen using (green) electrical energy. Essential for the performance of a PEM electrolysis cell are the flow dynamics of the so-called bipolar plates.

In this talk, we consider the topology optimization for the anode side bipolar plate of a PEM electrolysis cell by using the topological derivative. The goal of the optimization is to achieve a uniform flow distribution throughout the plate by taking aspects of manufacturability into account. Our approach gives rise to novel designs that could be used to improve the performance of PEM electrolysis cells.

Shape Optimization Algorithms in Banach Spaces

Pinzon Escobar, Jose Alfonso *(Universität Hamburg, Germany)*
Herbert, Philip *(Heriot-Watt University, United Kingdom)*
Siebenborn, Martin *(Universität Hamburg, Germany)*
Wollner, Winnifried *(Universität Hamburg, Germany)* 16:40

The main focus of this work is shape optimization in function spaces, particularly under partial differential equation constraints. We follow the recent trends in this area by proposing algorithms that find optimal solutions to problems in Banach spaces, as opposed to well-known approaches in Hilbert spaces. Our work is based on finding a descent direction in $W^{1,\infty}$ by approximating the solution to a corresponding constrained minimization problem. This is done, for instance, via the alternating direction method of multipliers. Building on previous work, we combine this with an optimization scheme based on a parameter-free approach.
We show results for fluid dynamics applications in which the target domain is optimized with

respect to the dissipation of energy. This is a well-known problem for which the optimal shape has a tip. The functional is constrained by the incompressible Navier-Stokes equations, and trivial solutions are avoided by imposing constraints on barycenter and volume. We present results for domains that require a high number of discrete elements to represent the target domain.
Their discretization implies that very-large systems of equations will be formed, some of which need to be solved several times within a optimization step.
Therefore, our case studies are computationally demanding, and the use of supercomputers is required.

Optimization of multiple non-smooth shapes based on a product shape manifold

Pryymak, Lidiya *(TU Bergakademie Freiberg, Germany)* 17:00
Suchan, Tim *(Helmut Schmidt University/University of the Federal Armed Forces Hamburg, Germany)*
Welker, Kathrin *(TU Bergakademie Freiberg, Germany)*

One way to interpret shape optimization is as the optimization on shape spaces. For fluid-mechanical problems a common occurrence is a shape that contains kinks. So far to the best of the author's knowledge no shape space with a Riemannian structure that contains non-infinitely-smooth shapes has been established, which inhibits the use of well-established gradient-based optimization methods on Riemannian manifolds. In this talk, a novel shape space that has a Riemannian manifold structure is proposed. The novel shape space can be used to optimize non-infinitely-smooth shapes, and additionally provides the possibility to optimize multiple shapes simultaneously.

Furthermore, numerical results for the minimization of viscous energy dissipation constrained by the Navier-Stokes equations, together with additional geometrical constraints enforced by an Augmented Lagrange method on the shape space are presented.

Eigenvalue optimization with respect to shape-variation in electromagnetic cavities

Herter, Christine *(Universtiät Hamburg, Germany)* 17:20
Wollner, Winnifried *(Universtiät Hamburg, Germany)*

In this talk we consider the optimization of particle accelerators in sense of eigenvalue optimization with respect to small shape-variations. The electromagnetic field and its associated eigenvalue are governed by the time-harmonic Maxwell's eigenvalue problem. We use a mixed weak formulation by Kikuchi (1987) and discretize the function spaces with a mixed finite element method by means of Nédélec and Lagrange elements. We formulate an optimization problem which is based on a method of mappings. To solve the constraining Maxwell's eigenvalue optimization problem, we calculate derivatives based on a method of adjoint calculus and introduce a damped BFGS method. We compare the numerical results with a gradient descent method.

A Novel Approach for Topology Optimization of Fluid Flow

Haubner, Johannes *(Universität Graz, Österreich)*
Ulbrich, Michael *(Technische Universität München, Deutschland)*
Neumann, Franziska *(Technische Universität München, Deutschland)*

17:40

A new approach for density based topology optimization is presented in the setting of Stokes flow. It is based on classical topology optimization and phase field approaches, and introduces a different way to relax the underlying infinite-dimensional mixed integer problem. We compare the novel approach to state-of-the-art density based and phase field approaches. Moreover, we discuss the connection to topological derivative based approaches. We give a theoretically founded choice of the relaxed problems. The density is modeled on a space that allows for jumps along hypersurfaces, such as BV or fractional order Sobolev spaces. Degrees of freedom in modeling the optimization problem are chosen based on theoretical considerations, i.e., by discussing the arising optimization problems concerning existence, differentiability and convergence towards solutions of the unrelaxed problem. Numerical results for the Stokes problem are presented. Moreover, in order to show the potential of the new approach, we do a comparison to a classical approach.

Preserving Mesh Quality in Shape Optimization

Onyshkevych, Sofiya *(University of Hamburg, Germany)*
Siebenborn, Martin *(University of Hamburg, Germany)*
Wollner, Winnifried *(University of Hamburg, Germany)*

18:00

In PDE-constrained shape optimization a lot of computational effort is used to update the geometry at every iteration step. This iterative process can result in loss of element quality and degeneracy, which is particularly relevant for applications involving large deformations of some parts of the domain. To avoid re-meshing we model the mesh deformation using the method of mappings. We use an extension equation that maps a boundary control variable to a deformation field defined over the entire domain. This allows us to reduce computational costs and promote the preservation of mesh quality. As the underlying model, we use the benchmark problem of minimizing the energy dissipation of an obstacle in a flow tunnel. By using the nonlinear extension operator proposed in our previous work, we increase the set of reachable shapes, allowing us to model large deformations. In this talk, we discuss how the choice of parameters of the extension equations affects the mesh quality. Further, we study the influence of the extension factor on the convergence properties of the iterative solvers by studying the condition number of the Hessian of the optimality system derived from the Lagrangian.

A Second-Order Method for Mesh Denoising and Inpainting

Baumgärtner, Lukas *(HU Berlin, Germany)*
Bergmann, Ronny *(NTNU Trondheim, Norway)*
Herzog, Roland *(Heidelberg University, Germany)*
Schmidt, Stephan *(HU Berlin, Germany)*
Vidal-Núñez, José *(University of Alcalá, Spain)*
Weiß, Manuel *(Heidelberg University, Germany)*

18:20

We present a novel approach to solve denoising and inpainting problems for surface meshes. The purpose of denoising is to remove geometric noise while preserving important features such as sharp edges, while inpainting refers to filling in missing parts of the geometry. A discrete variant of the total variation of the unit normal vector field serves as a regularizing functional to achieve both goals. In order to solve the resulting problem, we combine split Bregman (ADMM) iterations with a shape Newton method. Numerical examples are included demonstrating the performance of the method with some complex 3D geometries.

Asymptotically based optimization of flow-induced deformation of periodic flexural structures made of thin yarns

Krier, Maxime *(Fraunhofer ITWM, Kaiserslautern, Germany)*
Orlik, Julia *(Fraunhofer ITWM, Kaiserslautern, Germany)*
Pinnau, René *(RPTU, Kaiserslautern, Germany)*

18:40

The fluid-structure interaction problem of Stokes flow through a linear elastic, thin porous structure is considered. The micro-resolved structure is deterministic with an in-plane periodicity of ϵ and consists of long thin yarns in contact. It can be described by a handful of geometrical and mechanical parameters such as distances between yarns, friction coefficients, linear material properties and yarn cross-sections. Such problems typically arise e.g. in filtration applications with woven filter media.

Due to drastically differing length scales between fluid domain and the micro-resolved structure, direct numerical approaches for the problem are impractical in most scenarios.
Therefore an asymptotically derived model for the limit $\epsilon \to 0$ by means of two-scale convergence is considered. In the asymptotic limit, the problem is reduced to 3D Stokes flow coupled to a permeable 2D Kirchhoff plate with non-standard interface coupling: the plate's vibration is proportional to the pressure jump across the plate. The plate's effective elasticity tensors as well as its permeability are determined by auxiliary problems on the smallest periodic unit of the structure, so called cell problems.

In this presentation, an optimization problem of tracking type based on the asymptotic model is considered: The microscopic design of the structure is to be chosen such that a desired flow-induced deformation profile of the structure in steady-state is reached. The deformation profile is directly linked to the structure's filtration efficiency and is therefore of high interest in industrial application. The optimization problem is rigorously analyzed and an adjoint based optimization algorithm is derived. Details on the numerical implementation are given and the algorithm is exemplified for real-world woven filters.

S19-05: Optimisation of differential equations

Date: June 2, 2023 08:30-10:30
Room: HSZ/101

Derivatives and optimal control of a sweeping process

Brokate, Martin *(TU München, Germany)* 08:30

The sweeping process due to Moreau describes a specific form of a rate independent evolution. We present results on the directional derivatives of its solution operator and on an associated control problem.

An Optimal Design Problem for an Elastic Plate in a Dynamic Contact with an Obstacle

Bock, Igor *(FEI Slovak University of Technology, Slovak Republic)* 08:50

We deal with an optimal control problem governed by an initial-boundary value problem for a hyperbolic variational inequality describing perpendicular vibrations of an anisotropic elastic plate against a rigid obstacle. A variable thickness of a plate plays the role of a control variable. The state problem is not uniquely solved. In order to overcome the problem of *a priori* estimates of states we restrict the admissible set of states to solutions obtained through the penalization method. We verify the existence of an optimal thickness function and the generalized optimality conditions.

Optimal Control of Free Boundary Problems

Pinnau, René *(RPTU, Germany)* 09:10

In this talk we present FBPs in different areas of application, e.g. filter production, and the corresponding optimal control problems. These include the production of the fibre material as well as the control of the filtration process. The problems are analysed and we use the adjoint variables to derive the derivative information which is needed for the respective numerical solution. Further, we discuss possible relaxations and approximations.

Optimal Control of Free Boundary Problems

Zurloh, Corinna *(RPTU, Germany)* 09:30

We consider an optimal control problem constrained by a free boundary problem (FBP). FBPs have various applications such as in fluid dynamics, flow in porous media or finance. For this work we study a model FBP given by a Poisson equation in the bulk and a Young-Laplace equation accounting for surface tension on the free boundary. Transforming this coupled system to a reference domain allows to avoid dealing with form derivatives. However, this results in highly nonlinear PDE coefficients, which makes optimal control problem rather difficult. Therefore, we present a new relaxation approach by introducing the free boundary as a new control variable, which transforms the original problem into a sequence of simpler optimization problems without free boundary. Using asymptotic analysis, we show that a solution of the original problem can be indeed approximated in this way.

Network Boundary Control of the Semilinear Isothermal Euler Equation Modeling Gas Transport on a Network of Pipelines

Bongarti, Marcelo *(Weierstrass Institute for Applied Analysis and Stochastics, Germany)* 09:50
Hintermüller, Michael *(Weierstrass Institute for Applied Analysis and Stochastics, Germany)*

In this talk, we briefly discuss the analysis and tracking type optimal control of the nonlinear transport of gas in a network of pipelines. The gas distribution's evolution on a given pipe is modeled by an isothermal semilinear compressible Euler system in one space dimension. On the network, solutions satisfying (at nodes) the so-called Kirchoff flux continuity conditions are shown to exist within the vicinity of an equilibrium state. The nonlinear optimization problem then aims at driving such dynamics to a given target distribution by the means of suitable (network) boundary controls while keeping the distribution within given (state) constraints.

Uniform Turnpike Property and Singular Limits

Hernandez, Martin *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)* 10:10
Zuazua, Enrique *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany; Universidad Autónoma de Madrid, Spain)*

In the mathematical study of gas transport, as in several engineering areas, parameter-dependent models arise naturally to fit the reality to be represented. However, asserting a uniform property that satisfies the whole family of solutions of the parameter-dependent problem is not always straightforward. Motivated by singular limits in long-time optimal control problems, we investigate a class of parameter-dependent parabolic equations. First, we prove a turnpike result uniform with respect to the parameters of the equation within a suitable class. The main ingredient of our proof is the justification of the uniform exponential stabilization of the corresponding Riccati operators, which can be derived from the uniform null control properties of the model. As an application of this property, we focus on a rapidly oscillating heat equation. In the one-dimensional setting, we obtain a uniform turnpike property with respect to the highly oscillatory heterogeneous medium. Afterward, applying classical results from homogenization theory, we establish the homogenization of the turnpike property; that is, we can pass the limit in the optimal control variable while preserving the turnpike property. To the best of our knowledge, this is the first result related to singular limits in the turnpike context. Finally, numerical experiments validate the results.

S19-06: Optimisation of differential equations

Date: June 2, 2023 16:00-18:00
Room: HSZ/101

Optimal control of quasilinear parabolic PDEs with gradient terms and pointwise state-gradient-constraints

Bonifacius, Lucas *(n.a.)* 16:00
Hoppe, Fabian *(Deutsches Zentrum für Luft- und Raumfahrt DLR, Germany)*
Meinlschmidt, Hannes *(Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany)*
Neitzel, Ira *(Rheinische Friedrich-Wilhelms-Universität Bonn, Germany)*

This talk is concerned with optimal control of quasilinear parabolic PDEs with pointwise constraints on the gradient of the state. Besides applications requiring such type of constraints, the consideration of pointwise bounds on the gradient of the state can be motivated as follows: when including a semilinear term of order one, e.g., a quadratic gradient term, into the state equation, global-in-time existence of solutions to this equation cannot be proven anymore, in general. Interestingly, this issue can be overcome by imposing appropriate bounds on the gradient of the solution, i.e. by adding state-gradient-constraints to the control problem. For the resulting problem formulation we prove existence of optimal controls and derive first-order optimality conditions.

Space -time Variational Methods for Parabolic Optimal Control Problems

Reinhold, Alexander *(Ulm University, Germany)* 16:20
Beranek, Nina *(Ulm University, Germany)*

Optimal Control Problems with PDE constraints are not only highly relevant for a wide range of applications but also an interesting ongoing subject in research of numerical methods. In this talk we want to discuss Optimal Control problems where the constraint is a parabolic time dependent PDE. We might also consider additional constraints of the control in the form of box constraints. Usually these type of problems are solved using time stepping schemes to solve the constraining PDE and the arising adjoint equation. But lately approaches using simultaneous space-time discretizations are investigated. In this talk we will discuss the application of a space-time variational formulation for the optimal control problem. We will discuss the approach in the infinite dimensional setting using Bochner-Lebesgue spaces and derive the optimality system in this setting. Here we will focus especially on the handling of the arising adjoint equation. Furthermore, we want to show the differences of this method in comparison to classical semi discretization methods as well as to other space-time approaches. We show the application of a second order semi-smooth Newton method to solve the optimization problem and propose a discretization with a tensor type approach in space and time. An implementation to solve this system as well as numerical examples are presented. In an outlook we will show the potential and challenges of this approach w.r.t. Model Order Reduction for optimal control problems.

An Algorithmic Framework for Optimal Control of Hybrid Dynamical System with Parabolic PDEs

Kuchler, Christian *(Humboldt-Universität zu Berlin, Germany)* 16:40
Hante, Falk *(Humboldt-Universität zu Berlin, Germany)*

We present an algorithmic approach for the computational solution of optimal control problems with hybrid nature governed by linear parabolic PDEs featuring implicit switches. We discuss a step wise reformulation of the original formulation into a more tractable setting based on methods from disjunctive programming and a time transformation method. After removal of the implicit switching rule at the cost of the introduction of explicit switching variables and vanishing constraints, the connection of the resulting formulation to problems with equilibrium constraints is established and studied. The previous steps in combination with smoothening and a Moreau-Yosida type penalty approach allow the derivation of necessary first order optimality conditions to characterize candidates for optimality to the original system. Following the detailed discussion of each individual reformulation step, we introduce the algorithmic framework founded on a semismooth Newton method. Finally, we report on computational experiments and compare them in the light of the initial formulation.

Inverse optimal control in transportation networks

Schillinger, Thomas *(University of Mannheim, Germany)* 17:00
Göttlich, Simone *(University of Mannheim, Germany)*
Mehlitz, Patrick *(BTU Cottbus-Senftenberg)*

We present a bilevel optimization approach to the reconstruction of desired demands in optimal control problems over transportation networks of tree type via given noisy measurements. The network dynamics are described by a linear advection equation with individual speeds on each arc. At the sinks of the network unknown demands occurs.

On the lower level we aim to choose the inflow control such that the quadratic deviation of the supply and demand is minimized. The upper level problem is used to reconstruct the demands by choosing appropriate weights of given base demand levels.

First, the existence of optimal solutions associated with such hierarchical optimization problems is discussed in detail. Second, we investigate the numerical solution of the problem via a suitable discretization strategy and techniques from quadratic optimization. Third, some numerical experiments are presented to visualize variable features of the underlying model including different strategies of how to observe the network.

Parameter identification in piezoelectricity based on all-at-once and reduced regularization

Kuess, Raphael *(Humboldt-Universität zu Berlin, Germany)* 17:20

Piezoelectric devices have become indispensible in almost all households, industry and medicine with an applications range from mobile phones and Diesel fuel injectors to ultrasound imaging and dental scalers. Due to the upcoming switch to lead-free piezoceramics and the associated non-reproducible characterization of the material properties, the consistent and reproducible characterization of the material parameter set is of significant relevance for practical applications.

In this talk we will investigate the parameter identification problem for the piezoelectric partial differential equation using regularization based on all-at-once and reduced iterative methods. The choice of these formulations is of particular interest for nonlinear models, which is especially noticeable in computational aspects. Therefore, the procedure is based on modeling and solving these inverse problems in these different settings by fitting simulated experimental data. Furthermore, numerical examples will be provided.

A trust-region algorithm for parameter identification in multigroup pandemic models

Friedemann, Markus *(BTU Cottbus Senftenberg, Germany)* 17:40

Parameter identification for a nonlinear ODE describing a pandemic model is studied. In the model, the population is divided into several spatially separated subpopulations. Between those subpopulations, there is some (possibly infectious) contact due to traveling. The main goal is the identification of time-dependent contact parameters in the interaction terms between subgroups. The parameters can be considered in $L^2(0,T)$ and $H^1(0,T)$ to provide the possibility of regularizing the solution in the case of noisy data. Existence of solutions is proven and optimality conditions are discussed. A penalty approach is chosen to handle constraints. A solution algorithm based on a trust-region approach with Steihaug CG as an inner solver is introduced. Global and local convergence properties are investigated and fast local convergence is proven. Numerical results are presented.

S20: Dynamics and control

Organizer(s): **Matschek, Janine** *(U Magdeburg)*
Flaßkamp, Kathrin *(U Saarland)*

S20-01: Dynamics and control

Date: May 30, 2023 13:30-16:10
Room: HSZ/401

Online Learning for Control: Bringing Sequential Decision Making in the Loop

Iannelli, Andrea *(University of Stuttgart, Germany)* 13:30

The increase in systems complexity caused by societal challenges and the push to address more demanding tasks makes the synthesis of actions to achieve certain closed-loop system's performance a sequential decision-making problem under uncertainty. This motivates us to rethink the standard paradigm in control design of synthesizing the control algorithm offline (e.g. a matrix of transfer functions as in loop shaping). In this work we will present our ongoing work towards framing control of adaptive systems in changing environments as an online learning problem, whereby the decision-maker takes sequential decisions by solving a series of time-varying optimization problems having a-priori only partial knowledge of the cost functions. On the one hand, the online learning viewpoint inherently takes into account the time-varying and uncertain nature of the problem. On the other hand, it considers a different performance metric than those commonly used in system theory and control, i.e. regret, which measures the accumulated suboptimality with respect to a clairvoyant decision maker.

Motivated by the goal to understand what online learning, traditionally used in game-theoretic or decision-making problems which have no dynamics, can offer in the context of systems theory and control, we investigate here two control theoretic problems through the lens of online learning. First, we study under which conditions establishing certain rates of regret is equivalent to proving asymptotic stability of the underlying closed-loop system. It turns out that for linear (potentially time-varying) systems subject to adversarial disturbances and controlled by linear (potentially time-varying) state feedback policies linear regret implies asymptotic stability. Conversely, bounded input bounded state (BIBS) stability and summability of the state transition matrices imply linear regret.

Second, we consider the classical problem in inexact Model Predictive Control (MPC) of analyzing the closed-loop properties of a system controlled with an MPC controller which does not solve the online problem to optimality because it can only compute a finite number of iterative steps. We develop new results for characterizing transient performance and we show the connection between suboptimality in the standard sense and the regret associated with a clairvoyant decision maker that can take optimal actions at every step.

These findings further our understanding of the system theoretic meaning of widespread performance metrics in online learning. This is a pre-requisite for adopting design techniques from sequential decision making for synthesis of flexible and adaptive controllers which must be provably safe when they operate in dynamic environments.

Approximate Time Optimal Control by Deep Neural Networks Trained with Numerically Obtained Optimal Trajectories

Zauner, Christian *(Institute of Robotics, Johannes Kepler University Linz, Austria)*
Gattringer, Hubert *(Institute of Robotics, Johannes Kepler University Linz, Austria)*
Müller, Andreas *(Institute of Robotics, Johannes Kepler University Linz, Austria)*

14:10

This contribution focuses on online time optimal control of nonlinear systems. This is achieved by approximating the results of time optimal control problems (TOCP) with deep neural networks depending on the initial and terminal system state. In general, solving a TOCP for nonlinear systems is a computationally challenging task, especially in the context of nonlinear model predictive control (NMPC) with hard real time boundaries successful termination of a TOCP within sample times suitable for controlling mechanical systems cannot be guaranteed.

Therefore, our approach is to train three deep neural networks with different aspects of numerical solutions of TOCPs with random initial and terminal state. At first, it is tested whether the initial and terminal states are feasible by means that a trajectory from each state to an equilibrium state can be found, which satisfies all the system constraints. The results are used to train a neural network classifying a system state to be either feasible or infeasible. Then, if both are feasible, the TOCP is solved. By utilizing Bellman's principle of optimality, one optimal trajectory results in many optimal trajectories connecting different system state pairs along the trajectory. One neural network is then trained with the optimal time to get from one system state to another and one neural network is trained with the optimal system input, which has to be applied at a given system state to reach another state within minimal time.

If sufficiently trained, the network approximating the optimized system inputs can be used directly as nonlinear state dependent controller. Although this results in close to time optimal motion of the system, satisfying all constraints on the system states cannot be guaranteed in general. However, by using all three networks, the TOCP with varying time horizon of the time optimal NMPC can be approximated by a finite time horizon OCP. Thereby, the deviation of the system inputs from the values provided by the approximated optimal system inputs and the approximated time from the end of the fixed time horizon to the terminal state serve as cost function and the network classifying the feasibility of the system states serves as additional constraint. The so gained approximated NMPC law is guided by the approximated system inputs while satisfying the system constraints.

In order to verify this procedure by simulation, it is applied to a simple prove of concept example as well as the model of an industrial robot.

Towards neural network enhanced integrators for efficient lifetime assessment of wind energy converters

Othmane, Amine *(Saarland University, Germany)*
Flaßkamp, Kathrin *(Saarland University, Germany)*

14:30

In the near future, a significant portion of wind energy converters (WECs) installed in Germany and Europe will reach the end of design life, typically 20 years. For example, approximately half of the WECs installed in northeastern Germany will have reached their design life by 2025.

The implications of the current geopolitical and climate crises well highlight the potential issues resulting from a poor and slow energy transition. Therefore, there is a strong interest in operating existing WECs beyond their initially planned design life as long as safety requirements are met. In addition, considering the currently faltering expansion of wind energy in Germany, it is also desirable from an ecological point of view and in the interest of society to operate an existing turbine longer such that its full load-bearing capacity is utilized. Raw materials can be saved, waste is avoided, and the sustainability of renewable energy generation can ultimately be increased.

Guidelines for the lifetime extension of WECs require comparing design site conditions with real ones. For this purpose, numerical studies estimate fatigue effects by simulating models of WECs for a high number of different conditions, i.e., repeatedly solving differential equations. However, it is well known that the design of numerical integration schemes requires finding a compromise between computational burden and magnitude of approximation errors. This compromise is especially difficult when high-dimensional systems are considered for large time horizons.

This contribution investigates the use of neural networks (NNs) for the approximation of numerical integration errors. The residual elements will be learned using NNs and their approximations will be used to adapt the numerical schemes. The resulting integrators will be analyzed in numerical studies and their performances will be compared to those of well-established methods. The focus will especially be on computational burden. The analytical properties will be addressed in light of local errors and stability properties.

Remark: This contribution is part of the project "KIWi: KI-Simulationskorrekturen zur Laufzeitverlängerung von Windenergieanlagen" funded by the German Federal Ministry of Education and Research. The academic project partners are the Center for Industrial Mathematics (ZeTeM) at the University of Bremen and the Fraunhofer Institute for Wind Energy Systems.

On the approximability of Koopman-based operator Lyapunov equations

Breiten, Tobias *(Technische Universität Berlin, Germany)*
Höveler, Bernhard *(Technische Universität Berlin, Germany)*
14:50

Computing the Lyapunov function of a system plays a crucial role in optimal feedback control, for example when the policy iteration is used. This talk will focus on the Lyapunov function of a nonlinear autonomous finite-dimensional dynamical system which will be rewritten as an infinite-dimensional linear system using the Koopman operator. Since this infinite-dimensional system has the structure of a weak-* continuous semigroup in a specially weighted Lp-space one can establish a connection between the solution of an operator Lyapunov equation and the desired Lyapunov function. It will be shown that the solution to this operator equation attains a rapid eigenvalue decay, which justifies finite rank approximations with numerical methods. The usefulness for numerical computations will also be demonstrated with two short examples.

Finite-data error bounds for kernel-based approximations of the Koopman operator

Nüske, Feliks *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany)*
Peitz, Sebastian *(Paderborn University, Germany)*
Philipp, Friedrich *(Technische Universität Ilmenau, Germany)*
Schaller, Manuel *(Technische Universität Ilmenau, Germany)*
Worthmann, Karl *(Technische Universität Ilmenau, Germany)*

15:10

We consider the data-driven approximation of the Koopman operator on Reproducing Kernel Hilbert Spaces (RKHS). Our focus lies on two complementary scenarios: Independent and identically distributed data points and data collected from long-term ergodic trajectories. To obtain probabilistic bounds for the finite-data estimation error, we derive an exact expression for the variance of the kernel cross-covariance operator. Moreover, we derive a bound on the prediction error of observables in the RKHS by means of a finite Mercer series expansion. In case of Koopman-invariance of the RKHS, we provide bounds on the full approximation error. The theoretical results will be illustrated by means of an example with the Ornstein-Uhlenbeck processs.

Willems' fundamental lemma for linear descriptor systems

Faulwasser, Timm *(TU Dortmund, Germany)*
Schmitz, Philipp *(TU Ilmenau, Germany)*
Worthmann, Karl *(TU Ilmenau, Germany)*

15:30

The fundamental lemma by Willems et al. allows to completely describe all trajectories of a controllable linear time-invariant system based on a single trajectory with persistently exciting input. This result has profound implications for non-parametric modelling and data-driven control. We present a variant of the fundamental lemma tailored to regular linear descriptor systems and propose a data-driven framework for predictive control. We demonstrate the applicability using a benchmark example related to energy networks. Further, we give first thoughts towards a generalization to partial differential equations.

S20-02: Dynamics and control

Date: May 31, 2023 14:00-16:00
Room: HSZ/401

Sample efficiency in data-driven MPC and Reinforcement Learning

Peitz, Sebastian *(Paderborn University, Germany)* 14:00

As in almost every other branch of science, the advances in data science and machine learning have also resulted in improved modeling, simulation and control of nonlinear dynamical systems, prominent examples being autonomous driving or the control of complex chemical processes. However, many of these approaches face the issues that they (1) do not have strong performance guarantees and (2) often tend to be very data hungry. In this presentation, we discuss different approaches to improve the sample efficiency in data-driven feedback control. We address both model predictive control (MPC) as well as reinforcement learning (RL). In MPC, learning an accurate surrogate model is paramount for the performance. Exploiting techniques from mixed-integer control, we show that one can leverage performance guarantees of autonomous systems - which have been studied much more extensively - to obtain related error bounds for control problems. In RL, we address both the usage of surrogate models as well as the exploitation of system symmetries to improve sample efficiency. We demonstrate our findings using several example systems governed by partial differential equations.

Non-holonomic Systems: Geometry, Design of Predictive Controllers, and Remaining Difficulties

Ebel, Henrik *(University of Stuttgart, Institute of Engineering and Computational Mechanics)*
Rosenfelder, Mario *(University of Stuttgart, Institute of Engineering and Computational Mechanics)*
Eberhard, Peter *(University of Stuttgart, Institute of Engineering and Computational Mechanics)* 14:40

Non-holonomic systems, foremost in the form of vehicles such as cars, truck-trailer combinations, and baggage tugs, are indispensable in many applications. Yet, surprisingly, feedback control design for these systems remains a challenge. Just in recent times it has been commonly understood that classic design paradigms for model predictive control (MPC) can and will fail when trying to stabilize state set-points of even the simplest non-holonomic systems. Hence, to the knowledge of the authors, until very recently, there was no general procedure or even guideline on how to design functioning predictive controllers (without added terminal ingredients) for a wider set of non-holonomic systems. In this context, this work discusses a ready-to-apply MPC design procedure for driftless non-holonomic systems, which we recently proposed. The procedure facilitates nominal stability proofs, with the key ingredient being a non-quadratic cost function tailored to the control system's non-holonomic constraints. The

cost becomes more involved as the system's degree of non-holonomy increases. Formal guarantees rely on the (non-trivial) derivation of a homogeneous system approximation and recent MPC theory for (approximately) homogeneous systems. However, this does not provide any constructive intuition on why the tailored non-quadratic costs work. Thus, in this contribution, we provide novel, intuitive geometric insight on why the cost design fits the geometry induced by non-holonomic constraints. Following this, parking vehicles with MPC becomes a graspable example for sub-Riemannian geometry and the sub-Riemannian distance. Nevertheless, physical vehicles are never driftless since they are subject to inertia. While hardware experiments do show decent performance when governing real-world vehicles with a tailored drift-neglecting MPC controller, this contribution explicitly considers the physical second-order case. Moreover, despite its nice geometric interpretation, the comparatively involved non-holonomic MPC design procedure raises the question how well other feedback control techniques deal with such systems. To shed light on that question, we present empirical evidence from parking vehicles with reinforcement learning. Finally, we give an outlook to several aspects of the predictive control of non-holonomic systems that seem to remain unsolved, despite the real-world significance of such systems. The presented geometric insight may inspire their solution.

Funnel MPC

Dennstädt, Dario *(Universität Paderborn, Germany)* 15:00

Model Predictive Control (MPC) is nowadays a widely used control technique for linear and non- linear systems due to its ability to handle multi-input multi-output systems under control and state constraints. Given a model of the system, the idea is to predict the future system behavior and iteratively solve Optimal Control Problems (OCPs). To use a MPC algorithm initial and recursive feasibility have to be ensured and it is inherently necessary to have a sufficiently accu- rate model in order to compute an optimal control signal. A complementary control technique which does not rely on a model of the system but computes the control signal merely based on the current state of the system is funnel control. It is an adaptive high-gain output-error feedback controller. Under certain structural assumptions this concept guarantees the tracking of a prescribed reference signal within predefined bounds.

In this talk the novel concept *Funnel-MPC* (FMPC) is presented, which combines both approaches, i.e. Model Predictive Control and funnel control. The optimal control problem solved in each iteration of Funnel MPC resembles the basic idea of penalty methods used in optimization. Utilizing a stage cost design which mimics the high-gain idea of funnel control, this new approach allows guaranteed output tracking of smooth reference signals with prescribed performance for multi-input multi-output systems. This is achieved without imposing any terminal conditions or requirements on the length of the prediction horizon. While first results required the usage of output constraints in the optimal control problem, these restrictions were lifted in newer works. Most recent advances on Robust-FMPC allow for the application of Funnel MPC in the presence of unknown disturbances and even a structural plant-model mismatch. Future research aims to additionally incorporate learning techniques

to allow for steady improvement of the used model and, thus, controller performance while guaranteeing output tracking within predefined boundaries.

Recent progress on data-driven output feedback stochastic predictive control

Pan, Guanru *(TU Dortmund University, Germany)*
Ou, Ruchuan *(TU Dortmund University, Germany)*
Faulwasser, Timm *(TU Dortmund University, Germany)*
15:20

Commonly, Model Predictive Control (MPC) is based on the repeated solution of an optimal control problem. As such MPC usually relies on a *model* of underlying dynamics. However, there is a rapidly growing line of research which replaces the model with data-driven system descriptions. Of particular interest are methods which can work with input-output-data only. So far most of the research on data-driven predictive control has focused on noise-corrupted measurement data but not on the consideration of stochastic disturbances. In this talk, we discuss data-driven predictive control with stochastic uncertainties. We show how a tailored variant of the ubiquitous fundamental lemma in combination with polynomial chaos expansions enables data-driven output-feedback stochastic predictive control. We present sufficient conditions of stability and recursive feasibility through the design of initial conditions and terminal ingredients. Finally, we draw upon numerical examples to illustrate our findings.

A generalized stacked reinforcement learning method for sampled systems

Osinenko, Pavel *(Skolkovo Instite of Science and Technology, Moscow, Russia)*
Dobriborsci, Dmitrii *(Deggendorf Institute of Technology, Cham, Germany)*
15:40

Reinforcement learning approaches are commonly considered in the context of Markov decision processes (MDP), where the environment (the controlled dynamical system) is considered in discrete time. Some approaches, such as Q-learning, collapse altogether when the environment is time-continuous. However, the latter property is inherent in physical systems. In this report, we present an approach that applies to continuous-time environments which combines model-predictive control and Q-learning. The control is implemented in a sampled manner,i.e., holding actions over fixed periods of time steps. Such a setup is physically plausible given the digital nature of modern controllers. We provide optimality analysis and an experimental case study with a mobile robot. The results show high potentials of the new approach, called stacked Q-learning, compared to the model-predictive control baseline.

S20-03: Dynamics and control

Date: June 1, 2023 08:30-10:30
Room: HSZ/401

Time-Optimal Trajectory Planning of a Redundantly Actuated Planar Parallel Robot Driven with Series Elastic Actuators

Kordik, Thomas *(Institute of Robotics, Johannes Kepler University Linz, Austria)* 08:30
Zauner, Christian *(Institute of Robotics, Johannes Kepler University Linz, Austria)*
Marauli, Tobias *(Institute of Robotics, Johannes Kepler University Linz, Austria)*
Gattringer, Hubert *(Institute of Robotics, Johannes Kepler University Linz, Austria)*
Müller, Andreas *(Institute of Robotics, Johannes Kepler University Linz, Austria)*

Current research on parallel kinematic mechanisms (PKM) addresses the use of elastic components aiming at applications where well-defined physical compliance is important, e.g. human-robot interaction and rehabilitation. Redundant actuation of PKM is another research direction that was proposed to increase their dynamic capabilities and performance. This paper combines the two approaches and exploits them for time-optimal control.

The time-optimal control problem (OCP) for the point-to-point trajectory planning for non-redundantly and redundantly actuated PKM equipped with standard rigid drives as well as with series elastic actuators (SEA) is formulated. The OCP is implemented in MATLAB and solved numerically using the CasADi framework and IPOPT solver. Results are shown for a planar PKM with and without actuation redundancy when actuated with standard drives and with SEAs.

The dynamic model of the SEA-actuated PKM splits into two dynamical systems coupled by the elastic component of the SEA only. This control system is differentially flat with the end-effector coordinates as flat output. Consequently, the EE-trajectory needs to be four times differentiable with respect to time. The redundant actuation of the compliant PKM results in an additional degree of freedom, which allows preloading the elastic components without altering the EE-position. This enables the possibility to store and release potential energy at the starting and terminal points. In this case, the flat output consists of the EE-coordinates and an additional coordinate representing the preload. It is shown how this can be exploited to further optimize the trajectory.

Pareto-optimal primitives for graph-based motion planning

Pedrosa, Matheus V. A. *(Saarland University, Germany)* 08:50
Flaßkamp, Kathrin *(Saarland University, Germany)*

Classical continuous-time optimal control does not easily allow for switching objectives. Additionally, maintaining admissibility in highly constrained settings leads to computationally challenging up to intractable optimization problems. To circumvent these complexities, different graph-based planning techniques have recently been successfully applied to planning and control problems in autonomous driving.

The state space quantization for graph-based approaches can be based on motion primitives, which are segments of trajectories of a nonlinear system that can be concatenated. The concatenation rules are expressed as a directed graph, where the edges and vertices are two

special kinds of motion primitives. This promotes a trajectory generation with less computational complexity than solving motion planning as a nonlinear optimization problem. As a requirement, solving trajectory planning as a graph search requires an optimal path criterion, which is usually considered to be the shortest path. However, other criteria are of interest, too, for instance, the shortest time, the highest comfort, or the reduction of energy consumption. Then, in this work, we compute a set of optimal compromises, named Pareto set, such that the planning is not restricted to a single optimization criterion. For that, we compute Pareto-optimal motion primitives from a multiobjective optimal control problem. In parallel, structure-preserving primitives, named trim primitives, are equipped with unit costs.

The number of selected primitives leads to graphs of different sizes and is crucial for planning performance. Thus, we design a generalist graph which can then be shrunk to subgraphs on-the-fly, accordingly to, for example, restrictions from traffic rules, the profile of the passengers, or the driving mode. For instance, consider the vehicle's utility modes as "economy", "sport", and "off-road", or ambulances driving with or without sirens on. Numerical examples will picture the usage of this generalist graph composed of Pareto-optimal motion primitives.

Interplay of stage-cost design and discretization in optimal control of linear port-Hamiltonian systems

Şen, Gökçen Devlet *(Technische Universität Ilmenau; Istanbul Technical University)* 09:10
Schaller, Manuel *(Technische Universität Ilmenau)*
Worthmann, Karl *(Technische Universität Ilmenau)*

We consider the problem of optimal state transition with minimal energy. Here, we investigate the interplay of different state-cost designs and discretization. We show that in view of time discretization, the choice of theoretically equivalent costs matters. Furthermore, we consider the impact of additional regularization terms. While all cost functionals exhibit a turnpike property w.r.t. the non-dissipative subspace, the added regularization term leads to a considerable increase in energy consumption. Then, we extend our results to the tracking problem within model predictive control. Here, we show that state transition within the conservative subspace can be conducted very efficiently without quadratic control penalization.

Ellipsoidal Inter-Sample Collision Avoidance in Optimal Control

Herrmann-Wicklmayr, Markus *(Saarland University, Germany)* 09:30
Flaßkamp, Kathrin *(Saarland University, Germany)*

In optimal control problems, the geometry of objects e.g. for collision avoidance plays an important role. Often, these objects are described by simple approximations, such as polyhedra and ellipsoids. This work deals with collision avoidance of two ellipsoids. W.l.o.g., we assume one stationary and one moving ellipsoid. The collision avoidance is encoded as continuous-time constraints in the optimal control problem (OCP). When applying direct optimal control methods in order to transcribe to a static optimization problem, these constraints can only be enforced at finitely many time instances. Hence, it might occur that the continuous-time constraints are satisfied at two neighboring time instances, but are violated in between. Approaches to overcome this issue coined the term inter-sample collision/obstacle avoidance.

For the ellipsoidal case, we introduce linear morphing of the moving ellipsoid between two time instances, meaning we assume linear interpolation of center point and angle changes of the ellipsoid. Based on the collision test of Gilitschenski and Hanebeck (A Robust Computational Test for Overlap of Two Arbitrary-Dimensional Ellipsoids in Fault-Detection of Kalman Filters, 2012), we derive additional nonlinear constraints to be included in the static OCP. These additional constraints ensure that optimal solutions are guaranteed to avoid collisions of the ellipsoids at all times. The significance of the inter-sample collision avoidance constraints are demonstrated via a numerical example.

Turnpike property of mechanical systems

Flaßkamp, Kathrin *(Saarland University, Germany)*
Maslovskaya, Sofya *(Paderborn University, Germany)*
Ober-Blöbaum, Sina *(Paderborn University, Germany)*
Wembe, Boris *(Paderborn University, Germany)*
09:50

The turnpike property characterizes a quasi-static behavior of solutions of optimal control problems defined on a large time horizon. In this case, the solutions converge to a neighborhood of a steady state and stay there for a major part of the time interval. In many practical examples in mechanical and biological systems, the convergence is not towards a steady state but some attracting trajectory, though. It was recently shown that for the mechanical systems admitting a symmetry with respect to an abelian group action, these trajectories correspond to the relative equilibria of the system. In this talk we will show how this property of optimal control for mechanical systems generalizes to non abelian group actions.

Learning polynomial based approximation for optimal feedback control

Vasquez Varas, Donato *(Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences)*
Kunisch, Karl *(Johann Radon Institute for Computational and Applied Mathematics, Austrian Academy of Sciences; Institute for Mathematics and Scientific Computing, University of Graz)*
10:10

It is well known that the design of optimal feedbacks for high dimensional and non linear control problems is a difficult task, both from the computational and theoretical point of view. A classical approach for obtaining an optimal feedback law is based on dynamical programming. This requires to solve the Hamilton-Jacobi-Bellman equation, which it is known to suffer from the curse of dimensionality. In this work, we present an approach to obtain optimal feedback laws based on a learning task in the space of multivariate polynomials. We provide results concerning convergence and generalization power of the methodology. In addition, we performe some numerical experiments to ilustrate the capabilities of our approach.

S20-04: Dynamics and control

Date: June 1, 2023 16:00-19:00
Room: HSZ/401

Model order reduction strategies for interconnected systems with a large number of inputs and outputs

Aumann, Quirin *(University of Technology Chemnitz)* 16:00
Benner, Peter *(University of Technology Chemnitz; Max Planck Institute for Dynamics of Complex Technical Systems)*
Saak, Jens *(University of Technology Chemnitz; Max Planck Institute for Dynamics of Complex Technical Systems)*
Vettermann, Julia *(University of Technology Chemnitz)*

Interpolation-based data-driven methods, such as the Loewner framework, are established and effective approaches to find a realization of a dynamical system from measurements of the system's transfer function. If a system-theoretic representation of the original model is not available or unfeasible to evaluate efficiently, such reduced realizations enable effective analysis and simulation. A common issue of interpolation-based data-driven methods is that they do not enforce stability of the resulting surrogate model.

Numerical models of machine tools are an interesting engineering application for such data-driven methods. Thermo-mechanical finite element models predict the dynamic behavior of machine tool systems during the manufacturing process. Such models consist of interconnected substructures, which may or may not be moving relative to each other. An important quantity of interest is the displacement of the tool center point from its desired location due to mechanical deformation, which is mainly caused by the system's constantly changing thermal field. Numerical models describing the thermo-mechanical behavior of machine tools are typically very large, and methods to reduce their computational complexity are therefore required for their efficient application in design and control.

The substructures of machine tools may exhibit different properties, for example local nonlinearities, and may often be designed independently. Maintaining self-contained (reduced-order) models for the substructures enables a flexible design process, as new machine designs can efficiently be assembled by combining the substructures. However, such models often have a high number of inputs and outputs to correctly model their interconnections and couplings.

In this contribution, we use interpolation-based data-driven methods to compute surrogate models of thermo-mechanical numerical models of machine tools. Only transfer function evaluations are required for these methods. Therefore the approach can readily be integrated into workflows relying on proprietary simulation software where an extraction of system matrices required for classic (intrusive) projection-based model order reduction methods is often an involved process or even impossible. The resulting reduced-order models are required to preserve stability, as they should be used for time domain analysis. In particular, we study the intrinsic challenge for an effective model order reduction arising from the large amount of inputs and outputs of the subsystems.

Nonintrusive model order reduction for stochastic differential equations

Freitag, Melina *(University of Potsdam, Germany)*
Nicolaus, Martin *(University of Potsdam, Germany)*
Redmann, Martin *(University of Halle(Saale), Germany)*
16:20

In this work we aim to provide a nonintrusive model order reduction method in a noisy setting. Starting from linear and controlled stochastic differential equation with unknown coefficients, we infer a reduced order model purely from gathered data.
Based on developments in the field of operator inference, the drift is obtained by an least squares approach for the estimated expected value dynamics of the reduced model. The diffusion coefficients and covariance matrix of the generating Wiener process are computed by a square root free Cholesky factorization.
We provide numerical results for the case that the linear dynamics are given by a spatially discretized partial differential equation.

Time-Limited Balanced Truncation for Data Assimilation

König, Josie *(Universität Potsdam, Germany)*
Freitag, Melina *(Universität Potsdam, Germany)*
16:40

Balanced truncation is a well-established model order reduction concept in system theory that has been applied to a variety of problems. Recently, a connection between linear Gaussian Bayesian inference problems and the system theoretic concept of balanced truncation was drawn for the first time. Although this connection is new, the application of balanced truncation to data assimilation is not a novel concept: It has already been used in four-dimensional variational data assimilation (4D-Var) in its discrete formulation. In our work, the link between system theory and data assimilation is further strengthened by discussing the application of balanced truncation to standard linear Gaussian Bayesian inference, and, in particular, the 4D-Var method. Similarities between both data assimilation problems allow a discussion of established methods as well as a generalisation of the state-of-the-art approach to arbitrary prior covariances as reachability Gramians. Furthermore, we propose an enhanced approach that allows to balance Bayesian inference for unstable systems and improves the numerical results for short observation periods.

Discrete time scattering passive port-Hamiltonian systems

Cherifi, Karim *(TU Berlin, Germany)*
Gernandt, Hannes *(Fraunhofer Insititue for Energy Infrastructures and Geothermal Systems (IEG), Germany)*
Hinsen, Dorothea *(TU Berlin, Germany)*
Mehrmann, Volker *(TU Berlin, Germany)*
17:00

Passivity is usually defined, for linear dynamical systems, using quadratic supply rates such as impedance and scattering supply rates. Port Hamiltonian systems are a special type of passive systems. Most of the literature on linear port Hamiltonian systems focuses on continuous-time impedance passive systems. In this talk, the focus is on discrete-time scattering

passive systems that are also causal i.e. their solution does not depend on the future. We derive a port Hamiltonian representation for scattering passive causal dynamical systems and study the relation to bounded real transfer functions. The relation to passivity characterized by the Kalman-Yakubovich-Popov (KYP) inequality is also discussed. In addition, the relation between impedance and scattering passive systems is presented. Finally, we show how the time discretization of a continuous passive system falls into the class of discrete-time systems previously introduced.

Towards a modeling class for port-Hamiltonian systems with time-delay

Breiten, Tobias *(Technische Universität Berlin, Germany)*
Hinsen, Dorothea *(Technische Universität Berlin, Germany)*
Unger, Benjamin *(Universität Stuttgart)*
17:20

The framework of port-Hamiltonian (pH) systems is a powerful and broadly applicable modeling paradigm. In this talk, we extend the scope of pH systems to time-delay systems. Our definition of a delay pH system is motivated by investigating the Kalman-Yakubovich-Popov inequality on the corresponding infinite-dimensional operator equation. Moreover, we show that delay pH systems are passive and closed under interconnection.

An Embedding Observer for Nonlinear Dynamical Systems with Global Convergence

Gerbet, Daniel *(TU Dresden, Germany)*
Röbenack, Klaus *(TU Dresden, Germany)*
17:40

State observers are widely used to recover the internal state of a dynamical system from the systems output trajectory, which is usually only a projection of the full state. While there is a relatively straight way to do this for a linear system, the observer design becomes more difficult for nonlinear systems. Not all such systems can be immersed into the observer canonical form, where the observer design becomes as easy as in the linear case. A different approach is to construct an observer based on the observability normal form, known as a high-gain observer.

Although whence a nonlinear system is globally observable, it may not suffice to construct a state observer with the same dimension as the systems state space. This is because higher order derivatives of the output trajectory may be required in order to distinguish different system states. Furthermore, the vector field for the system in observability normal form is not necessarily Lipschitz continuous everywhere, a condition required for global convergence of the high-gain observer.

In this contribution we show a direct method that allows to embed an autonomous polynomial system into its observability normal form, where the map is locally invertible except at the not locally observable points, and is globally invertible for every globally observable system. By possible further increasing the dimension of the observers state space the corresponding vector field may become Lipschitz continuous such that the high-gain observer with guaranteed convergence can be designed. The inverse mapping extended to the whole observer state space yields a projection onto the state space of the system to be observed.

An approach to non-linear observer design via optimal control theory - the Mortensen observer

Schröder, Jesper *(Technische Universität Berlin, Germany)*
Breiten, Tobias *(Technische Universität Berlin, Germany)*
18:00

Many real processes can be described by mathematical models. Since these representations are based on idealized assumptions and simplifications, it is nearly impossible to describe any system perfectly. Another problem arises from the fact that often the state of the actual system is not available, and instead only an output can be obtained. Examples of such an output are measurements by devices like microphones and heat sensors, which are subject to additional noise. One approach to recovering an approximation of the state of the system is to design a dynamical observer. While the Kalman filter offers an efficient solution to this problem for linear systems, the design of non-linear observers is still challenging. This talk gives an introduction to the minimum energy estimator, also called the Mortensen observer, which was proposed among others by R. E. Mortensen in 1968. The method approaches the problem via optimal control theory. We discuss feasible assumptions to ensure the well posedness of the resulting observer equation, which is achieved by a sensitivity analysis of the corresponding value function. Here, the associated Hamilton-Jacobi-Bellman equation plays an integral part. Numerical experiments illustrate the theoretical result.

The effect of model uncertainties in the reinforcement learning based regulation problem: an experimental case study with inverted pendulum

Pal, Amit Kumar *(Ruhr-Universität Bochum, Germany)*
Oveisi, Atta *(Ruhr-Universität Bochum, Germany)*
Nestorović, Tamara *(Ruhr-Universität Bochum, Germany)*
18:20

This work aims to improve the classical white-box model of an inverted pendulum in order to reach a more accurate representation of an actual pendulum on a cart system. The purpose of the model is to train different controllers based on machine learning algorithms. In the context of this paper, the inverted pendulum system is driven by a belt drive that is controlled by a stepper motor. Due to the nature of the controller, the input to the stepper motor is in the form of a non-smooth bang-bang-like signal that moves the cart to left, right, or terminates its movement. One of the main challenges, in this case, is to find a proper function to model the stepper motor as its dynamics cannot be captured with a constant gain. It has been shown that the transient behavior of the stepper motor when changing direction or stopping is not negligible in the closed-loop control performance. Accordingly, a grey-box scheme, which accounts for the uncertainties that are not included in the vanilla white-box model, is utilized to achieve a lower model mismatch compared to the actual pendulum.

Initially, the equation of motion was derived using the Euler-Lagrange equation with force on the cart as the control input. But in the real-time experiment, the interface is realized by the stepper motor's frequency modulator, hence a transfer function representing the relationship between the frequency and the force applied on the cart (in the model) is calculated as a black-box model. To improve the accuracy of the transfer function, an experimental data-driven design of this function is performed based on modern schemes in system identification, and the acquired data is utilized in two identification methods: (1) linear subspace

algorithm based on predictive error method (2) Nonlinear AutoRegressive with eXternal input model. For this purpose, the applied frequency to the stepper motor and the states from the actual system are recorded. Then, the applied force on the cart is calculated using the equation of motion and the recorded states. Additionally, the stiffness and damping coefficients in the white-box model have been shown to have a nonlinear dependency on the position and its rate. This dependency is captured by means of lookup table membership functions. Finally, it is shown that the frequency-force transfer function uncertainty due to exogenous disturbances is non-negligible and with the aim of having a more accurate model, an artificial neural network is introduced.

Catalog of Dynamical System Models

Fiedler, Julius *(TU Dresden, Institute of Control Theory, Germany)* 18:40
Knoll, Carsten *(TU Dresden, Institute of Control Theory, Germany)*

Dynamical system models play an important role in control engineering, both in research as well as in teaching. This is especially true when considering mechanical systems. In this contribution we present a catalog of - from a control theoretical point of view - relevant system models, that can be the subject of in depth analysis and used as benchmark systems or exercise material.

Our approach differs from similar works such as [1], in three key aspects: Firstly, we are not only providing the necessary equations to describe the model, but also offer an implementation of the model, that can be used both for symbolic analysis as well as numeric simulation and validation of e.g. a designed controller. Secondly, we characterize each model by means of semantically structured meta data. Thirdly, our catalogue (and its supporting software) is based on open repositories and thus can be incrementally improved and extended.

Our model implementations provide a homogeneous interface, that can be used for a variety of applications, from simulation to observer design or feedback control. The catalog is therefore useful as a benchmark to increase reproducibility of results of publications. It is also possible to automatically check the models in the catalog for specific control theoretic properties. E. g. we can automatically examine properties such as strong local accessibility or static input-to-state-linearizability.

The mentioned meta data relies on the Ontology of Control Systems Engineering (OCSE) [2]. System models are tagged with attributes, that then itself have semantic relations between each other, which allows for a high-resolution-classification of the entries in the catalog. therefore one can search the catalog for models with specific properties (e.g. strong local accessibility) and characteristics (e.g. a single input, or state dimension $n \geq 4$), without knowing the names of the system models.

The catalog is an open-source project containing over 30 system models of different domains; a significant part being non-trivial (underactuated) mechanical systems such as inertia wheel pendulum, triple pendulum on cart, four-bar linkage, and gantry crane.

Literatur

[1] Murray, Richard M and Rathinam, Muruhan and Sluis, Willem: Differential Flatness of Mechanical Control Systems: A Catalog of Prototype Systems, 1995

[2] Knoll, C.: Ontology of Control Systems Engineering (OCSE) — Source Code Repository, https://github.com/ackrep-org/ocse, 2022.

S20-05: Dynamics and control

Date: June 2, 2023 08:30-10:30
Room: HSZ/401

Application of feedforward and funnel feedback control to underactuated multibody systems

Drücker, Svenja *(Hamburg University of Technology, Germany)* 08:30
Berger, Thomas *(Paderborn University, Germany)*
Lanza, Lukas *(Ilmenau University of Technology, Germany)*
Reis, Timo *(Ilmenau University of Technology, Germany)*
Seifried, Robert *(Hamburg University of Technology, Germany)*

Underactuation occurs naturally in the design of many mechanical systems, such as lightweight machines, many types of cable-driven manipulators or flexible joint robots. These systems have more degrees of freedom than independent control inputs. With the development of new mechanical designs and functionalities, new control strategies must be designed accordingly in order to meet accuracy requirements. For underactuated systems, it is usually not possible to control all degrees of freedom independently and therefore, trajectory tracking control of such systems is a challenging problem.

This contribution analyzes a two degree of freedom control strategy applicable to tracking problems for underactuated systems. The control strategy combines funnel feedback control with feedforward control based on servo-constraints.

The servo-constraints approach is a model-based strategy to compute an inverse model of a multibody system. It can be computed in real-time and can be directly used as a feedforward controller. This methodology has shown to be an efficient control strategy for complex underactuated multibody systems. The remaining tracking error is usually small and can be compensated by a suitable feedback strategy. Here, funnel control is applied in the feedback loop. Funnel control is an adaptive output feedback control strategy. It is a model-free strategy and therefore robust against parameter and model uncertainties. Funnel control guarantees a prescribed performance of the tracking error.

The methodology is analyzed for two application examples. First, simulation results are shown for a mass-on-car system. The results show that the combination of servo-constraints with funnel control can reduce spikes in the feedback control and therefore reduce loads on the mechanical parts of the underactuated system. As a second application example, a torsional oscillator with two rotating disks is considered. Experimental results are presented to show that the proposed control strategy can reduce time lag and a steady state error compared to using only feedback control.

Overall, the results show that the combination of servo-constraints with funnel feedback control retains the advantages of both individual methods.

Stability and performance analysis of controlled brake system considering delayed actuator dynamics and communication delay

Horváth, Ádám *(Department of Railway Vehicles and Vehicle Structure Analysis, Budapest University of Technology and Economics, Műegyetem rkp. 3., H-1111 Budapest, Hungary)*
Béda, Péter *(Department of Railway Vehicles and Vehicle Structure Analysis, Budapest University of Technology and Economics, Műegyetem rkp. 3., H-1111 Budapest, Hungary)*

08:50

Efficiency and safety are key aspects of research and development in the automotive sector. On the field of commercial vehicles, these two keywords might be the most important. These vehicles have relatively high gross weight, and are able to participate in the traffic with more or less the same speed as smaller cars. Commercial vehicles are equipped with electro-pneumatic brake systems. These systems have many advantageous properties, but they require external energy input to be able to produce compressed air. In addition, there is time-delay in the system, that can cause performance and stability issues during braking. The main aim of this study is to analyze the effect of time-delay in electro-pneumatic brake systems considering different control strategies. There could be different origins of time-delay. Firstly, compressed air needs to travel from the reservoirs through valves, chokes and pipes to reach the brake chamber. As the velocity of the air is finite, pneumatic time-delay appears. The length of this delay depends on different physical and structural parameters of the system, such as the length of the pipes. As friction could be significant in the brake chamber and the caliper, a minimal value of pressure increment could be defined that is able to cause increment of the brake torque. Therefore, an additional part of the delay is caused by the time that needs to build up this minimal pressure. Modern brake systems are electronically controlled, there are several advanced functionalities implemented in them, such as anti-lock system (ABS), electronic stability program (ESP), etc. As commercial vehicles are relatively large vehicles, communication subsystems are required to deliver information between components far from each other. Therefore, communication delay appears in the electronic part of the system. A trade-off must be defined in connection with time-delay. Permanently decreasing time-delay might affect efficiency and costs of the system negatively. Deeper understanding of the effect of time-delay can provide basis of different structural modifications or application of advanced control techniques that makes the system robust under larger time-delay. A quarter-car model with different tire models is coupled with the dynamical system of the actuator that contains time delays. Slip control, wheel deceleration control and vehicle deceleration control strategies are applied to the vehicle system. Based on the structure of the controller, delay differential equations (DDE), neutral delay differential equations (NDDE) and DDEs with both neutral and advanced terms appear. Stability and performance characteristics are investigated.

An Approach to Agile Maneuvering with Hydrobatic Micro Underwater Robots

Alff, Thies Lennart *(Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TUHH), Germany)*
Seifried, Robert *(Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TUHH), Germany)*
Duecker, Daniel A. *(Institute of Mechanics and Ocean Engineering, Hamburg University of Technology (TUHH), Germany; MIRMI - Munich Institute of Robotics and Machine Intelligence, Technical University of Munich (TUM), Germany)*

09:10

Maritime environmental field exploration and monitoring are among the most promising tasks to be addressed by autonomous underwater vehicles (AUVs). While full-scale underwater robots are mostly deployed in ocean- and open water-like settings, the recently developed class of small scale micro AUVs (μAUV) enables accessing new confined and cluttered scenarios. Given the strict constraints on the vehicle size, the onboard computational and sensory resources of these vehicles are naturally limited. Hence, a key design criterion for any algorithm to be developed is being computationally light-weight. Following this thought, μAUVs pose much different requirements than ocean-going robots, as these focus on long planning horizons, own comparably slow dynamics, and carry sophisticated sensing equipment. Closing the loop from the original tasks of field exploration and monitoring, both constitute high-level planning tasks that are usually performed with slow update rates due to their strong computational requirements. Their output is often realized as a sequence of way points. On the other end of the system pipeline, we see there are high-rate low-level control schemes that drive the vehicle attitude toward its desired orientation. A desirable approach is, thus, to design a trajectory generation module that acts as an interface between both ends, taking, for instance, way points from the high-level planner as input while providing feasible setpoints at a high rate for the low-level controller. This approach considers the dynamic capabilities of the underwater robot while at the same time considering potentially present obstacles and avoiding those at a planning stage. This contribution exploits the synergies between aerobatic unmanned aerial vehicles (UAVs) and hydrobatic μAUVs: the concept of computational efficient trajectory generation for quadcopters in [1] is transferred to the underwater domain. However, the differences in modeling the vehicle's dynamics have to be considered and addressed by the proposed planning method with respect to (i) computational efficiency, (ii) robustness of the trajectory tracking performance, and (iii) the sampling strategy. The performance is evaluated in simulation and lab experiments yielding promising results. It is shown that the tracking performance can be improved by extending the implicit feedback control scheme in [1] by a dedicated tracking controller in the presence of uncertain hydrodynamic damping.

[1] Mueller, M.W.; Hehn, M.; D'Andrea, R.: A computationally efficient motion primitive for quadrocopter trajectory generation. IEEE Transactions on Robotics, Vol. 31, No. 6, p. 1294-1310, 2015.

Modeling and parameter identification for agricultural machines

Simonelli, Ruggero *(University of bremen, Germany)*
Büskens, Christof *(University of bremen, Germany)*
09:30

A series of technical and socialaspects have led the pressure to increase energy efficiency and reduce the level of environmental impact in agricultural production. Crop producers and equipment manufacturers have identified computerized assistance in operation management as an indispensable tool to optimize agricultural processes. A central place is occupied in this regard by the so called *digital twins,* computer models of a specific instance of an object or system which are also capable of exchanging data with the physical counterpart and updating their state accordingly. The core of a *digital twin* is given by the *digital mock-up,* or *offline digital twin,* that is the computer model of the system's physics. The goal of this work is to present the development of an *offline digital twin* for a novel *gantry-tractor* type autonomous agricultural machine. The peculiarity of this system resides in its until now scarcely adopted mechanical design and its ability to perform a range of processes by attaching different modules to its frame. After a brief introduction into the characteristics of a *gantry-type* tractor and its role in the context of *precision autonomous agriculture* and *Controlled Traffic Farming*, different components of the machine and dynamic phenomena are separately investigated and mathematically modeled. Particular focus is placed thereby on the study of the vehicle's lateral and longitudinal dynamics. Based on the software implementation of the mathematical models the unknown parameters are estimated by means of nonlinear optimization techniques, using sensor data collected during operation as the measurement reference: the accuracy of different estimation methods is evaluated against experimental samples collected by sensors. As a result a global model of the vehicle's dynamics is realized. In the end, the obtained model is coupled to the 3D CAD model and integrated in the ROS2/GAZEBO simulation environment, which also comprises the actual autonomous navigation software modules .

An adaptive scheme for the optimization of damping positions in vibrational systems

Przybilla, Jennifer *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Ugrica, Matea *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Truhar, Ninoslav *(Department of Mathematics, J.J. Strossmayer University of Osijek, Croatia)*
Benner, Peter *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
09:50

In this work, the problem of optimizing damping positions in vibrational systems is investigated. The objective is to determine the positions of external dampers in such a way that the influence of external excitations on the system is minimized. The energy response serves as an optimization criterion, whose computation involves solving Lyapunov equations. Hence, to find the best positions, many of these equations need to be solved, so that the minimization

process can have a high computational cost. To accelerate the process of finding the optimal positions, we propose a new reduction method. Our algorithm generates a basis spanning an approximation to the solution space of the Lyapunov equations for all possible positions of the dampers. We derive an adaptive scheme that generates the reduced solution space by adding the subspaces of interest, and then we define the corresponding reduced optimization problem that is solvable in reasonable amount of time. We decouple the solution spaces of the problem to obtain a space that corresponds to the system without external dampers and serves as a starting point for the reduction of the optimization problem. In addition, we derive spaces corresponding to the different damper positions that are used to expand the reduced basis if needed. Our new technique produces a reduced optimization problem of significantly smaller dimension that is faster to solve than the original problem, which we illustrate with some numerical examples.

A trajectory based study of mixing processes in closed and open flow systems

Klünker, Anna *(Leuphana University of Lüneburg, Germany)* 10:10
Padberg-Gehle, Kathrin *(Leuphana University of Lüneburg, Germany)*

The analysis and control of mixing in fluid flows has numerous applications. Recently, network based or trajectory based methods have been developed to study the coherent behavior in fluid flows. Here, we extend a trajectory based method using diffusion maps [1] to model and study the mixing of two types of fluids.

We consider closed and specific open flow systems, which present (idealized) models of mixing devices. These open systems are characterized by constant in- and outflow of fluid particles. Here, the chaotic saddle and its stable and unstable manifolds organize the transport and mixing processes. Particles near the stable manifold stay longer in the system and follow the unstable manifold on their way out [2].

In example systems, we study the resulting mixing patterns and quantify the mixing results by several mixing measures.

References

[1] Banisch, Ralf, and Koltai, Péter. “Understanding the geometry of transport: Diffusion maps for Lagrangian trajectory data unravel coherent sets.” *Chaos: An Interdisciplinary Journal of Nonlinear Science* 27.3 (2017): 035804.
[2] Aref, Hassan, et al. “Frontiers of chaotic advection.” *Reviews of Modern Physics* 89.2 (2017): 025007.

S20-06: Dynamics and control

Date: June 2, 2023 16:00-18:00
Room: HSZ/401

Sample-and-hold funnel control

Lanza, Lukas *(TU Ilmenau, Germany)* 16:00
Dennstädt, Dario *(University of Paderborn, Germany)*
Worthmann, Karl *(TU Ilmenau, Germany)*
Trenn, Stephan *(University of Groningen, Netherlands)*
Schaller, Manuel *(TU Ilmenau, Germany)*

Consider the classical control task of tracking a given reference trajectory with the output of a dynamical system, e.g., a robotic manipulator in a production line. Adding the requirement that the tracking must be done with prescribed accuracy, the well-known funnel controller is a suitable control technique. A peculiarity of the high-gain adaptive funnel control method is that the feedback law does not involve knowledge of the system to be controlled; only structural assumptions are made. Continuously receiving the system's output signal the funnel controller generates an input signal, which achieves output reference tracking with prescribed accuracy; namely, the tracking error is bounded away from the given funnel boundary. Note that the control signal is generated by using the continuously measured output. However, most control units are equipped with computers, so that neither the signals are measured continuously, nor the resulting control signals are.

In the present work we propose a novel sample-and-hold controller, which achieves output reference tracking with prescribed accuracy like the continuous funnel controller. Sample-and-hold here means that we consider the situation where the system's output signal is sampled only at discrete points in time, and these discrete-time measurements are used to compute a piecewise constant input value that is then applied until the next sampling time point. We show that the application of this controller yields a closed-loop initial value problem, which has a solution and all signals are bounded; moreover, the tracking error evolves within predefined boundaries. Note that from the existing literature on high-gain feedback control it is not obvious that such a control law exists and is successful. We highlight three aspects of the present contribution: we explicitly compute a globally valid sampling time, the resulting control signal is bounded and its bound can be computed in advance, and unlike to the existing funnel control results we allow that the initial error starts at the funnel boundary.

Control-Oriented Models for the Shallow Water Equations using Energy-Conserving Higher Order Discretization Schemes

Mayer, Luca *(UMIT TIROL, Austria)* 16:20
Wurm, Jens *(UMIT TIROL, Austria)*
Woittennek, Frank *(UMIT TIROL, Austria)*

The well-known Saint-Venant equations are often used to model shallow water in open channels. These open-channel problems are, for example, irrigation channels with rectangular cross-sections of the river bed [1-3]. Another application of the shallow water equations is the

modeling of snow avalanches [4, 5]. In [6, 7] control design for shallow water waves in a tube with a moving boundary and an arbitrary cross-section has been considered. Such feedback laws may require an observer to obtain the complete system state from certain point measurements. Important ingredients of such observers are accurate numerical models suitable for real-time implementation. These models rely on an appropriate discretization of the original spatially distributed model. In order to retain the stability properties of the latter model, energy-based methods are most appropriate when deriving the approximation. This actual contribution deals with higher-order approximation schemes for the system considered in [8], i.e., a boundary-actuated 1D shallow-water model with moving boundary and arbitrary cross-section. To cope with the time-varying spatial domain, the model equations are formulated using material fixed coordinates, i.e., Lagrange coordinates. As the distributed shallow-water model can be derived using the principle of least action (cf. [8, 9]), the action functional constitutes the starting point also for the derivation of the lumped approximation, i.e., the lumped parameter model. To this end, the action functional is discretized w.r.t. space on a material fixed grid. Afterward, the finite-dimensional model is derived by applying an appropriate quadrature scheme. Due to the fact, that the conservation of mass is taken into account as an auxiliary condition, the resulting model is a system of semi-explicit differential-algebraic equations (DAE). In contrast to (cf. [8]) within the actual contribution, higher-order quadrature formulae are employed. Although this is expected to deliver more accurate numerical approximations, the scheme results in more involved nonlinear DAE. Within the contribution, different approaches are discussed for the numerical solution of these DAE.

Prescribed finite-time stabilization for flat systems

Irscheid, Abdurrahman *(Saarland University, Germany)* 16:40
Rudolph, Joachim *(Saarland University, Germany)*

In many cases, asymptotic stabilization of a system does not suffice to meet time constraints, which has motivated methods for achieving so-called finite-time stability. This means that the solutions of a stable system converge to the equilibrium in a finite time. If, additionally, the settling time is uniformly bounded by a parameter independent of the initial conditions (ICs), the equilibrium is said to be fixed-time stable. These concepts have been extensively studied within the framework of linear and nonlinear systems (see, e.g., [3]). Moreover, prescribed-time stabilization, as originally introduced in [4], allows the terminal time to be prescribed independently of ICs and parameters. The main idea relies on so-called blow-up functions and a rigorous Lyapunov analysis. Alternatively, prescribed finite-time stabilization can also be motivated on the basis of time-scale transformations [1, 2]. This perspective allows for a straightforward generalization to flat nonlinear systems and boundary controlled distributed-parameter systems. This work presents a modular derivation of controllers for flat systems that stabilize a tracking error in prescribed finite time. For that, a class of linear time-varying differential equations with prescribed finite-time stability of the origin is derived via pole placement in the transformed time. As a consequence of flatness, the closed-loop dynamics of a controlled system can be chosen to belong to the derived system class. The resulting input signals are shown to remain bounded and satisfy smoothness requirements. Furthermore, the control strategy is inherently robust w.r.t. model uncertainties. It is also shown

that the method can be applied to an infinite-dimensional setting in a quite straightforward way. The proposed tracking controller is validated in a simulation of a kinematic car model as well as a boundary controlled partial differential equation.

References

[1] Y. Chitour, R. Ushirobira, and H. Bouhemou. Stabilization for a perturbed chain of integrators in prescribed time. SIAM J. Control Optim., 52:1022-1048, 2020.
[2] A. Irscheid, S. Bleymehl, and J. Rudolph. Prescribed finite-time stabilization for flat systems (in German). at - Automatisierungstechnik, 69:585-596, 2021.
[3] A. Polyakov, D. Efimov, and W. Perruquetti. Finite-time and fixed-time stabilization: Implicit Lyapunov function approach. Automatica, 51:332-340, 2015.
[4] Y.-D. Song, Y.-J. Wang, J.-C. Holloway, and M. Krstic. Time-varying feedback for regulation of normal-form nonlinear systems in prescribed finite time. Automatica, 83:243-251, 2017.

Input-to-state stability of a time-invariant system with control delay and additive disturbances

Ursu, Ioan *(National Institute for Aerospace Research Ëlie Carafoli= INCAS Bucharest, Romania)*
Toader, Adrian *(National Institute for Aerospace Research Ëlie Carafoli= INCAS Bucharest, Romania)*
Tecuceanu, George *(National Institute for Aerospace Research Ëlie Carafoli= INCAS Bucharest, Romania)*
Enciu, Daniela *(National Institute for Aerospace Research Ëlie Carafoli= INCAS Bucharest, Romania)*

17:00

In this paper a class of linear time invariant system with control delay and additive disturbances is considered. A state predictive feedback method is first applied to compensate the actuator delay. In this way, a closed loop system free of delay is achieved. The technique of construction of Lyapunov-Krasovskii functionals is briefly reviewed. It allows to ensure input-to-state-stability of the closed loop system. Applications are given for the lateral stability of an airplane with two controls, on the aileron and on the direction, in correlation with compliance with some regulatory flight conditions.

Frequency-dependent Switching Control for Disturbance Attenuation of Linear Systems

Zhang, Jing Jing *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany; Shanghai University, Shanghai, China)*
Heiland, Jan *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany)*
Benner, Peter *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany)*
Du, Xin *(Shanghai University, Shanghai, China)*

17:20

The generalized Kalman-Yakubovich-Popov lemma as established by Iwasaki and Hara in 2005 marks a milestone in the analysis and synthesis of linear systems from a finite-frequency perspective. Given a pre-specified frequency band, it allows to design passive controllers with excellent in-band disturbance attenuation performance at the expense of some of the out-

of-band performance. With that, one may define controllers that perform particularly well in a frequency range of interest. This paper focuses on control design of linear systems in the presence of disturbances with non-strictly or non-stationary limited frequency spectrum. We first propose a class of frequency-dependent excited energy functions as well as frequency-dependent excited power functions, which possess a desirable frequency-selectiveness property with regard to the in-band and out-of-band excited energy as well as excited power of the system. Based upon a group of frequency-selective passive controllers, we then develop a frequency-dependent switching control (FDSC) scheme that selects the most appropriate controller at runtime. We show that our FDSC scheme is capable to approximate the solid in-band performance while maintaining acceptable out-of-band performance with regard to global time horizons as well as localized time horizons. The method is illustrated by a commonly used aircraft benchmark model.

Fixed-Order H-infinity Control of Port-Hamiltonian Systems

Schwerdtner, Paul *(Technische Universität Berlin)*
Voigt, Matthias *(UniDistance Suisse)*
17:40

The H-infinity optimal control problem plays an important role in attenuating undesired external noise and dealing with model uncertainties in dynamical systems. Solving this problem classically is based on determining solutions of multiple algebraic Riccati equations. This approach often suffers from numerical difficulties, in particular in the vicinity of the optimal performance level. Furthermore, if the underlying system dynamics is of high complexity, then the controller is of the same order as the plant model which is undesired from the practical point of view. Therefore, we propose a new approach for port-Hamiltonian plant models for which we construct low-order port-Hamiltonian controllers. Using a structured parametrization of the controller we can connect the H-infinity control problem to a regression-type optimization problem based on frequency domain samples of the plant model. This strategy is particularly well-suited for large-scale systems and does not suffer from the problems of the Riccati equation approach.

S21: Mathematical signal and image processing

Organizer(s): **Brandt, Christina** *(U Hamburg)*
Schmitzer, Bernhard *(U Göttingen)*

S21-01: Mathematical signal and image processing

Date: May 30, 2023 13:30-16:10
Room: HSZ/201

Dynamical vs. variational perspectives in shape spaces and the flow of diffeomorphisms

Wirth, Benedikt *(Uni Münster, Germany)* 13:30

A shape space is a set of shapes (e.g. shapes of organs in computational anatomy or of animated characters in geometry processing) equipped with the structure of a Riemannian manifold. To compute distances, interpolating and extrapolating paths (and many other objects) in such a shape space one can follow the variational paradigm of minimizing the path energy or path length among all paths connecting two given shapes or alternatively the dynamical paradim of time-integrating the dynamical system associated with shortest paths (so-called geodesics). Depending on the context, one perspective may be more natural than the other. I will give an introduction to both paradigms and then present a variational approach to the theory and numerics of a specific, important shape space (or rather preshape space), the flow of diffeomorphisms or LDDMM space, which is traditionally treated from the dynamical perspective. The material will be based on joint work with Mara Guastini and Martin Rumpf.

Discrete Geodesic Calculus in the Manifold of Sobolev Curves

Hartwig, Florine *(University of Bonn, Germany)*
Rumpf, Martin *(University of Bonn, Germany)*
Wirth, Benedikt *(University of Münster, Germany)* 14:10

The infinite-dimensional manifold of closed, parametric immersed curves has been studied intensively with applications in shape analysis and medical imaging. This nonlinear space equipped with the second-order Sobolev metric is geodesically and metrically complete and there exist geodesic paths between two arbitrary curves in the same connected component. In this talk we derive a consistent discretization of the Riemannian calculus on this space of curves. To this end, we study a variational time discretization of geodesics based on a suitable Galerkin approach that prove the convergence to solutions of the time continuous problem. For the spatial discretization we represent closed curves by Fourier components. This leads to a fully practical scheme allowing us to efficiently compute discrete geodesics, a discrete exponential map, and a discrete parallel transport on the space of curves.This is based on joint work with Martin Rumpf, and Benedikt Wirth.

Data-driven reduced order modeling framework using nonlinear dimensionality reduction

Mjalled, Ali *(Chair of Automatic Control and System Theory, Ruhr University Bochum, Germany)* 14:30

Şereflioğlu, Mustafa *(Chair of Automatic Control and System Theory, Ruhr University Bochum, Germany)*
Torres, Edgar *(Chair of Automatic Control and System Theory, Ruhr University Bochum, Germany)*
Mönnigmann, Martin *(Chair of Automatic Control and System Theory, Ruhr University Bochum, Germany)*

Reduced order modeling (ROM) is a technique used to reduce the computational complexity of mathematical models by using a simplified description of the high-fidelity model. This can be achieved by identifying and representing the most important features of the system using a reduced basis that captures the essential modes of the system. Established ROM methods, for instance, Galerkin-projection, approximate the solution by linearly projecting high-dimensional spaces to a lower-dimensional space spanned by the reduced basis. However, the accuracy of these methods may be insufficient for complex and multiscale simulations due to the restriction to a linear space [1]. Alternatively, autoencoders can be used for nonlinear dimensionality reduction. Autoencoders train a neural network to reconstruct the original data from a low-dimensional vector, known as the latent vector, which represents a compressed version of the original space. In contrast to POD, autoencoders can capture more complex relationships and are well-suited for problems that have a nonlinear structure [2]. In light of this, we combine nonlinear dimensionality reduction techniques with time series prediction to build data-driven ROMs [3]. The presented framework consists of two-level neural networks. The high-dimensional space is nonlinearly compressed in the first level using the encoder function of the autoencoder. Subsequently, the temporal evolution of the latent vector is predicted in the second level. The original solution can be easily reconstructed using the decoder function of the autoencoder. In comparison with the projection-based ROM, i.e., POD with Galerkin-projection, this framework allows naturally to include parameters in the prediction without nonlinear interpolation of the POD basis [4]. We demonstrate the framework on a two-dimensional flow field simulation around circular bodies parametrized with the inlet fluid velocity. Results show that the developed data-driven ROM was able to successfully predict the dynamics of the flow for an unseen simulation.

[1] Berner, M.O., Scherer, V., and Monnigmann, M. (2020). Controllability analysis and optimal control of biomass drying with reduced order models. *Journal of Process Control.*

[2] Masci, J., Meier, U., Ciresan, D., and Schmidhuber J. (2011). Stacked convolutional Auto-encoders for Hierarchical feature extraction. *Proceedings of the 21st international conference on artificial neural networks.*

[3] Pant, P., et al. (2021). Deep learning for reduced order modelling and efficient temporal evolution of fluid simulations.

[4] Reineking, L., et al. (2022). Long-term stable reduced models for hydraulic systems governed by Reynolds averaged Navier-Stokes equations. *3th IFAC Symposium on Dynamics and Control of Process Systems.*

Parametrizing Product Shape Manifolds by Composite Networks

Sassen, Josua *(University of Bonn)*
Hildebrandt, Klaus *(TU Delft)*
Wirth, Benedikt *(University of Münster)*
Rumpf, Martin *(University of Bonn)*

14:50

Parametrizations of data manifolds in shape spaces can be computed using the rich toolbox of Riemannian geometry. This, however, often comes with high computational costs, which raises the question if one can learn an efficient approximation by a neural network. In this talk, we will show that this is indeed possible for shape spaces with a special product structure, namely those smoothly approximable by a direct sum of low-dimensional manifolds. Our proposed architecture leverages this structure by separately learning approximations for the low-dimensional factors and a subsequent combination. After developing the approach as a general framework, we will apply it to a shape space of discrete surfaces. Here, typical examples of data manifolds are given through datasets of articulated models and can be factorized, for example, by a Sparse Principal Geodesic Analysis (SPGA). We will demonstrate the effectiveness of our proposed approach with experiments on synthetic data as well as manifolds extracted from data via SPGA.

LiDAR based object detection for agricultural robots

Stronzek-Pfeifer, David *(University of Bremen, Germany)*
Patel, Shruti *(University of Bremen, Germany)*
Christof, Büskens *(University of Bremen, Germany)*

15:10

Light Detection and Ranging**(**LiDAR) sensors have proven to be a valuable tool to gather geometric information about the environment and are a crucial component in perception of autonomous systems. In the agricultural domain State-Of-The-Art algorithms for detection, classification and tracking often utilize a combination of LiDAR and camera by fusion of semantic and geometric information. This is in part due to the availability of fast algorithms specifically optimized to make use of the convenient 2D data structure of RGB-images. Still there are limitations relying on cameras in agriculture since they highly depend on favorable lighting conditions and generally lack explicit geometric information, while LiDAR is especially advantageous in that regard as well as regarding range. This makes LiDAR particularly valuable for perception applications such as self-localization, mapping, or object detection. The unstructured nature of 3D LiDAR point clouds, however, coupled with their possibly large size and density, presents a significant hurdle in terms of real-time capability for these kind of tasks. Object detection on 3D LiDAR sensor data is therefore challenging with density based clustering approaches (e.g. DBSCAN) being currently the most prominent and robust algorithms here. Yet solutions in agriculture usually are tied to very narrow use cases or rigorous down sampling to ensure real-time applicability which is not favorable. Here we will present a pipeline featuring ground segmentation (RANSAC) and clustering (DBSCAN) to exemplify the limitation of neighborhood search based approaches and show an alternative algorithm featuring 2.5D map representations to avoid the computational drawbacks and ensure real-

time capability. We utilize established algorithms to project the 3D LiDAR data into two distinct maps, a XY-map (birds eye view) and a YZ-map (field of view). Our approach is then to apply object detection algorithms on each of those maps individually and to further combine the information into a joint estimate. Hence the computational bottleneck shifts from handling unordered 3D LiDAR data to the fixed and predefined resolution of the aforementioned maps. From the information stored in the 2.5D map Axis Aligned Bounding Boxes (AABB) for each object are computed containing information about the objects position and dimensions which can be further used as input for tracking algorithms. We will compare the two approaches regarding its real-time capabilities for different domain specific use cases with simulated and real data from agricultural fields. Further we highlight methods for AABB fitting and evaluate an optimal map resolution.

Measurement methods in digital images of high-speed recordings for a quantitative vibration analysis of flame pulsations

Morich, Julian Andreas *(TU Dresden, Germany)*
Günther, Stefan *(TU Dresden, Germany)*
Odenbach, Stefan *(TU Dresden, Germany)*

15:30

Flame pulsations in combustion chambers can cause (economical) high damage, if the oscillation frequency of the flame corresponds to a natural frequency of the surrounding components. A targeted optimization of vibration-critical facilities requires a precise knowledge of the oscillating gas column. Various optical methods exist, to investigate vibrating flame problems and characterize their parameters. In case of consisting boiler systems with pulsation problems a high-speed vision by suitable cameras is the most promising approach. Due to the high time resolution of the image sequences the oscillation can be reconstructed. The perspective into a boiler system with a camera is highly challenging, since the count of revision openings is restricted and often unfavorable positioned. For this reason, the captured images underlying to a few disturbance variables, which have to be suppressed previously. This includes e.g. the varying background, which must be separated off to the flame. The restricted camera perspective leads to an optical distortion, which must be take into account. To investigate various effects on measuring flame vibrations, two test rigs were used. By a modified and modular camera system datasets were measured under laboratory conditions. Optical problems are examined with a real burner, which was installed into a boiler system. The image processing methods were tested in advance on a flameless analogue model. By use off different image processing methods for preprocessing and feature extraction a robust and suitable approach for analysis was developed. The introduced methods allow by the use of a sufficient fast camera and appropriate optics the insitu measurement of flames and the characterization of their oscillation parameters. Furthermore the measuring limit was shown just like a procedure to measure under difficult framework conditions.

S21-02: Mathematical signal and image processing

Date: May 31, 2023 14:00-16:00
Room: HSZ/201

Approximation of functions by short exponential sums

Plonka-Hoch, Gerlind *(University of Göttingen, Germany)* 14:00

We consider function approximation using short exponential sums of lengh with pairwise distinct complex frequencies. The exponential sum model can be well applied to periodic as well non-periodic function approximation. However, exponential decay of approximation errors in finite intervals and on R_+ has been shown only for special completely monotonic functions, while numerical experiments show very good approximation results also for other functions as Bessel functions or the Gaussian function. There are several algorithms around to obtain exponential sum approximations. Beside the very expensive generalized Remez algorithm there exist different suboptimal algorithms based on Prony's method, which employ function values, derivative values or moments of the function to be approximated. Further, there is a close connection between rational approximation in frequency domain and the approximation by exponential sums in spatial domain. In the talk, we give a survey on recents results on function approximation by exponential sums and corresponding numerical algorithms.

L^1-data fitting for Inverse Problems with subexponentially-tailed data

Meth, Kristina *(Julius-Maximilians-Universität Würzburg, Germany)*
Werner, Frank *(Julius-Maximilians-Universität Würzburg, Germany)* 14:40

Outgoing from [HW14] and [KWH16] we analyze variational regularization with L^1-data fidelity. We investigate discrete models with regular data in the sense that the tails decay subexponentiallly. Therefore, error bounds are provided and numerical simulations of convergence rates are presented.

[HW14] T. HOHAGE AND F. WERNER, Convergence rates for inverse problems with impulsive noise, SIAM J. Numer. Anal., 52 (2014), pp. 1203-1221.
[KWH16] C.KÖNIG, F. WERNER, AND T. HOHAGE, Convergence rates for exponentially ill-posed inverse problems with impulsive noise, SIAM J. Numer. Anal., 54 (2016), pp. 341-360.

Inexact proximal Langevin sampling

Kuger, Lorenz *(FAU Erlangen-Nürnberg, Germany)*
Ehrhardt, Matthias *(University of Bath, UK)*
Schönlieb, Carola-Bibiane *(University of Cambridge, UK)* 15:00

In order to solve advanced tasks like uncertainty quantification or hypothesis tests in Bayesian imaging inverse problems, we have to draw samples from the arising posterior distribution. For the usually log-concave but high-dimensional posteriors, Markov chain Monte Carlo methods based on time discretizations of Langevin diffusion are a popular tool. If the potential defining the distribution is non-smooth, as is the case for many relevant imaging problems, these discretizations are usually of an implicit form. This leads to Langevin sampling algorithms that require the evaluation of proximal operators, which is, for some of the potentials

relevant in imaging problems, only possible approximately using an iterative scheme. We investigate the behaviour of a proximal Langevin algorithm under the presence of errors in the evaluation of the proximal mappings. We generalize existing non-asymptotic and asymptotic convergence results of the exact algorithm to our inexact setting and quantify the additional bias between the target and the algorithm's stationary distribution due to the errors. We show that the additional bias stays bounded for bounded errors and converges to zero for decaying errors in a strongly convex setting. We apply the inexact algorithm to sample from the posterior of typical imaging inverse problems in which we can only approximate the proximal operator by an iterative scheme and validate our theoretical convergence results.

Rebricking frames and bases

Fink, Thomas *(University of Passau, Germany)*
Forster-Heinlein, Brigitte *(University of Passau, Germany)*
Heinrich, Florian *(University of Passau, Germany)* 15:20

In 1946, Dennis Gabor introduced the analytic signal $f+iHf$ for real-valued signals f. Here, H is the Hilbert transform. This complexification of functions gives access to their amplitude and phase information and has ever since given well-interpretable insight into the properties of the signals over time. The idea of complexification has been reconsidered with regard to many aspects: Multi-dimensional versions via the Riesz-Transform, in combination with multi-resolution approaches leading to Riesz wavelets, or the dual tree complex wavelet transform, and others.
In this context, we ask two questions:

- Which pairs of real orthonormal bases, Riesz bases, frames and Parseval frames $\{f_n\}_n$ and $\{g_n\}_n$ can be "rebricked" to complex-valued ones $\{f_n+ig_n\}_n$?
- And which real operators A allow for rebricking via the ansatz $\{f_n+iAf_n\}_n$?

In the presentation, we answer these questions and give a characterization which linear operators A are suitable for rebricking while maintaining the structure of the original real valued family. Surprisingly, the Hilbert transform is not among them.

Efficient Data Optimisation for Polyharmonic Inpainting with Finite Elements

Chizhov, Vassillen Mihailov *(Mathematical Image Analysis Group, Saarland University, Germany)* 15:40

Polyharmonic inpainting with optimised data has been used extensively in image reconstruction literature. We improve the quality and efficiency of the reconstruction in several ways. In order to decrease runtime, we replace the standard finite difference method with a finite element discretisation, adapted to a judiciously chosen form of the polyharmonic boundary value problem. This allows us to use linear triangle elements instead of relying on mixed formulations, discontinuous Galerkin discretisations, or complex high order elements. The resulting formulation is numerically advantageous and it easily generalises to high polyharmonic orders. Furthermore, we propose efficient data optimisation algorithms, which produce better quality reconstructions and are several orders of magnitude faster than current state-of-the-art methods. All of this allows us to work with very large images, which has been impractical using prior approaches.

S21-03: Mathematical signal and image processing

Date: June 1, 2023 08:30-10:30
Room: HSZ/201

Modeling Large-scale Joint Distributions and Inference by Randomized Assignment

Boll, Bastian *(Heidelberg University, Germany)* 08:30
Schwarz, Jonathan *(Heidelberg University, Germany)*
Gonzalez-Alvarado, Daniel *(Heidelberg University, Germany)*
Sitenko, Dmitrij *(Heidelberg University, Germany)*
Petra, Stefania *(Heidelberg University, Germany)*
Schnörr, Christoph *(Heidelberg University, Germany)*

We propose a novel way of approximating energy-based models by randomizing the parameters of assignment flows, a class of smooth dynamical data labeling systems. Our approach builds on averaging flow limit points within the combinatorially large simplex of joint distributions. In an initial learning stage, the distribution of flow parameters is selected to match a given energy-based model. This entails the difficult problem of estimating model entropy which we address by differentiable approximation of a bias-corrected estimator. The model subsequently allows to perform probabilistic inference by computationally efficient draws of structured integer samples which are approximately governed by the energy-based target Gibbs measure in the low-temperature regime. We conduct a rigorous quantitative assessment by approximating a small two-dimensional Ising model and find close approximation of the combinatorial solution in terms of relative entropy which outperforms a mean-field approximation baseline.

Quantum State Assignment Flows

Schwarz, Jonathan *(Heidelberg University, Germany)* 08:50
Boll, Bastian *(Heidelberg University, Germany)*
Sitenko, Dmitrij *(Heidelberg University, Germany)*
Gonzalez-Alvarado, Daniel *(Heidelberg University, Germany)*
Gärttner, Martin *(Heidelberg University, Germany)*
Albers, Peter *(Heidelberg University, Germany)*
Schnörr, Christoph *(Heidelberg University, Germany)*

We extend the assignment flow approach from categorial distributions to complex-valued hermitian density matrices, used as state spaces for representing and analyzing data associated with vertices of an underlying graph. Determining the flow of the resulting dynamical system by geometric integration causes an interaction of these non-commuting states across the graph, and the assignment of a pure (rank-one) state to each vertex after convergence. Some experiments with toy systems indicate the potential of the novel approach for data representation and analysis.

Splines in Wasserstein Spaces and Application to Texture Interpolation

Justiniano, Jorge Andres *(Universität Bonn, Germany)* 09:10
Rumpf, Martin *(Universität Bonn, Germany)*
Erbar, Matthias *(Universität Bielefeld, Germany)*

This talk introduces a time discrete variational model for splines in Wasserstein spaces to interpolate textures encoded as empirical probability measures. Cubic splines in Euclidean space are known to minimize the integrated squared acceleration subject to a set of interpolation constraints. As generalization on the space of probability measures the integral over the squared acceleration is considered as a spline energy and regularized by addition of the usual action functional. Both energies are then discretized in time using local Wasserstein-2 distances and the generalized Wasserstein barycenter. The existence of time discrete regularized splines for given interpolation conditions is established. The computation of time discrete splines is implemented numerically, based on entropy regularization and the Sinkhorn algorithm. A variant of the iPALM method is applied for the minimization of the fully discrete functional. A variety of numerical examples demonstrate the robustness of the approach and show striking characteristics of the method. The approach is used to interpolate synthesized textures. To this end a generative model for texture synthesis from a single sample image is taken into account and splines in Wasserstein space are used to generate spline interpolations of underlying feature distributions.
This is a joint work with Matthias Erbar and Martin Rumpf

Trigonometric Approximations of the Sparse Super-Resolution Problem in Wasserstein Distances

Catala, Paul *(University of Osnabrück, Germany)* 09:30
Hockmann, Mathias *(University of Osnabrück, Germany)*
Kunis, Stefan *(University of Osnabrück, Germany)*
Wageringel, Markus *(University of Osnabrück, Germany)*

This work considers the recovery of an arbitrary measure on the d-dimensional torus, given trigonometric moments up to degree n. Considering the convolution of the measure with powers of the Fejér kernel, which can be computed efficiently from the truncated moment sequence, we provide rates of convergence of the resulting polynomial density towards the measure in the p-Wasserstein distance, as the degree n increases. In particular, we show that the best possible rate for polynomial approximation is inversely proportional to the degree, and that it is achieved by adequately choosing the power to which the kernel is raised. Finally, we introduce another class of polynomial approximations, similar although not based on convolution, that converge pointwise to the characteristic function of the support of the measure. This is joint work with Mathias Hockmann, Stefan Kunis and Markus Wageringel.

The genetic column generation algorithm for multi-marginal optimal transport

Penka, Maximilian *(Technische Universität München, Germany)*
Friesecke, Gero *(Technische Universität München, Germany)*
09:50

We extended the recently introduced genetic column generation algorithm for multi-marginal optimal transport from symmetric to general problems. In my talk, I will first briefly introduce the multi-marginal optimal transport problem, starting from the well-known two-marginal case. The theoretical focus will be on sparsity results, which are essential for the following part. In the second part I will explain the Genetic Column Generation Algorithm and show its applications in the context of Wasserstein barycenters and splines, which can be used to interpolate images.

Multi-level Geometric Optimization

Müller, Sebastian *(Heidelberg University, Germany)*
Zisler, Matthias *(Heidelberg University, Germany)*
Petra, Stefania *(Heidelberg University, Germany)*
10:10

We propose a geometric multi-level optimization method that smoothly incorporates constraints. Specifically, we formulate the constraints as a Riemannian manifold, defined as the parameter space of a distribution family, using the Fisher-Rao metric. Similar to Euclidean smooth unconstrained multi-level optimization, we define a hierarchy of geometric models with varying discretization levels. Finer models provide high accuracy but are expensive to compute, whereas coarser models are less accurate but computationally efficient. Our approach speeds up fine level updates by computing the search direction based on a coarser model. Moreover, the multi-level optimization method preserves feasibility of the updates by leveraging the Riemannian geometry induced by the hierarchy. We extend classical components of multi-grid methods to the Riemannian structure of our constraints. We show that the proposed algorithm is well suited to large-scale ill-posed image reconstruction problems.

S21-04: Mathematical signal and image processing

Date: June 1, 2023 16:00-19:00
Room: HSZ/201

Solving linear inverse problems with invertible residual networks

Arndt, Clemens *(Universität Bremen, Germany)* 16:00
Denker, Alexander *(Universität Bremen, Germany)*
Dittmer, Sören *(Universität Bremen, Germany)*
Heilenkötter, Nick *(Universität Bremen, Germany)*
Iske, Meira *(Universität Bremen, Germany)*
Kluth, Tobias *(Universität Bremen, Germany)*
Maass, Peter *(Universität Bremen, Germany)*
Nickel, Judith *(Universität Bremen, Germany)*

Data-driven solution techniques for inverse problems, typically based on specific learning strategies, exhibit remarkable performance in image reconstruction tasks. These learning-based reconstruction strategies often follow a two-step scheme. First, one uses a given dataset to train the reconstruction scheme; often, one parameterizes this scheme via a neural network. Second, the reconstruction scheme is applied to a new measurement to obtain a reconstruction. We also follow these steps but parameterize the reconstruction scheme with an invertible residual network. We demonstrate that the invertibility opens the door to new investigations into the influence of the training and the architecture on the resulting reconstruction scheme. The investigations reveal a formal link to the regularization theory for linear inverse problems.

A method development for the extraction of particle traces in fast X-Ray micro tomography by utilising motion artefacts

Siebert, Judith Marie Undine *(TU Dresden, Germany)* 16:20
Odenbach, Stefan *(TU Dresden, Germany)*

We developed a method for the tracing of particle movement with fast X-Ray micro tomography under laboratory conditions. The examination of opaque filtration systems is usually not trivial, but µCT offers a possibility to examine the inside of systems in a non-destructive way. With their high brilliance and resolution synchrotron systems provide the best data, however they are hardly available. Therefore, the focus lays on laboratory CT systems such as the in-house and self-built µCT system we used. In order to investigate particle movement in opaque systems, reduced and 3D printed pore systems with a pore diameter of 2 mm as well as a one way vessel and a vessel for sedimentation experiments have been created. In those filter structures glycerine as medium and barium titanate spheres as particles were used. Since the minimum time for a 360 ° µCT scan is 30 s, the filtration experiments meaning the particle movement took place during an active scan causing parabolic and irregular motion artefacts. Furthermore, due to detector specifications, shorter scan times result in fewer and therefore noisier data. For the evaluation we used digital image processing with Python. In order to determine the particle trace through the system it turned out to be the best option to

exploit the motion artefacts. As a result of the motion artefacts being irregular in shape and intensity we use a combination of random sample consensus (RANSAC) algorithm and the method of least squares to fit ellipses onto every artefact. To determine the particle position the best ellipse in every layer is chosen and the apices of the parabola shaped artefacts are determined. Combing the coordinates of every image layer to a trace allows it to reconstruct what path the particle chose. The results show that with the developed method it is generally possible to determine the particle coordinates and therefor reconstruct a trajectory of particles in the range of 200-600 µm. The quality of the found coordinates highly depends on the quality of the data and the curvature of the artefact.

Inversion of the Modulo Radon Transform via Orthogonal Matching Pursuit

Beckmann, Matthias *(University of Bremen, Germany)* 16:40

In the recent years, the topic of high dynamic range (HDR) tomography has started to gather attention due to recent advances in the hardware technology. The issue is that registering high-intensity projections that exceed the dynamic range of the detector cause sensor saturation, which, in turn, leads to a loss of information. Inspired by the multi-exposure fusion strategy in computational photography, a common approach is to acquire multiple Radon Transform projections at different exposure levels that are algorithmically fused to facilitate HDR reconstructions.

As opposed to this, a single-shot alternative to the multi-exposure fusion approach has been proposed in our recent line of work which is based on the Modulo Radon Transform, a novel generalization of the conventional Radon transform. In this case, Radon Transform projections are folded via a modulo non-linearity, which allows HDR values to be mapped into the dynamic range of the sensor and, thus, avoids saturation or clipping. The folded measurements are then mapped back to their ambient range using reconstruction algorithms.

In this talk we introduce a novel Fourier domain recovery method, namely the OMP-FBP method, which is based on the Orthogonal Matching Pursuit (OMP) algorithm and Filtered Back Projection (FBP) formula. The proposed OMP-FBP method offers several advantages; it is agnostic to the modulo threshold or the number of folds, can handle much lower sampling rates than previous approaches and is empirically stable to noise and outliers. The effectivity of the OMP-FBP recovery method is illustrated by numerical experiments.

This talk is based on joint work with Ayush Bhandari (Imperial College London).

A projection-based approach to extend digital volume correlation for 4D spacetime measurements

Kosin, Viktor *(ENS Paris Saclay, France; Leibniz Universität Hannover, Germany)*
Fau, Amélie *(ENS Paris Saclay, France)*
Jailin, Clément *(GE Healthcare, France)*
Smaniotto, Benjamin *(ENS Paris Saclay, France)*
Wick, Thomas *(ENS Paris Saclay, France; Leibniz Universität Hannover, Germany)*
Hild, François *(ENS Paris Saclay, France)* 17:00

In-situ (tomography) experiments are generally based on scans reconstructed from a large number of projections acquired under constant deformation of samples. Standard digital

volume correlation (DVC) methods are based on a limited number of scans due to acquisition duration. They thus prevent analyses of time-dependent phenomena. In this presentation, a modal procedure is proposed that allows time-dependent occurrences to be analyzed. It estimates spacetime displacement fields during the whole loading history. The spatial modes are based on standard DVC, which is subsequently enriched using projection-based digital volume correlation (P-DVC) to measure the temporal amplitudes. The method is applied to two cases, namely, a virtual experiment mimicking wedge splitting and an actual shear test on a pantographic metamaterial inducing large motions. With the proposed method, the temporal amplitude in the real test was measured for each projection leading to a temporal resolution of one tenth of a second and the analysis of 16,400 time steps. For the proposed algorithm, the sensitivity to the acquisition angle of the sample was investigated and measurement uncertainties were assessed.

S21-05: Mathematical signal and image processing

Date: May 31, 2023 08:30-09:30
Room: HSZ/201

A Mean-Field Optimal Control Approach to the Training of NeurODEs & AutoencODEs

Cipriani, Cristina *(Technical University of Munich, Germany)* 08:30

NeurODEs are a specific type of neural networks which contain shortcut connections that allow interpreting their training as a stochastic optimal control problem. Our work is twofold: first we consider the mean-field version of the problem and derive first order optimality conditions in the form of a mean-field version of the Pontryagin Maximum Principle. Our result is based on a novel and generalized version of the Lagrange multiplier theorem on convex sets of spaces of measures and it provides a unique control solution, which is also Lipschitz continuous.

On the other hand, we focus on the particle version of the problem and extend this well-known model to the case of Autoencoders. For this kind of networks we provide a novel architecture and an alternative training method based on the Pontryagin Maximum Principle. For both the applications, we show some explanatory and easy-to-read numerical examples which give powerful insights into the resulting algorithm.

The Geometry of Adversarial Training

Bungert, Leon *(Hausdorff Center for Mathematics, University of Bonn, Germany)* 08:50

In this talk I will speak about adversarial training (AT)—a succesful method for the training of adversarially robust classifier. It turns out to be equivalent to a variational geometric regularization problem involving a nonlocal perimeter. Using this structure one can show that AT admits a convex relaxation which is reminiscent of the Chan-Esedoglu model from image denoising and allows to prove existence of solutions. Combing techniques from Gamma-convergence and inverse problems one can also study the asymptotic regularization effect of AT in the limit of a vanishing adversary.

This is joint work with Nicolás García Trillos, Ryan Murray, and Kerrek Stinson.

p-Laplacian Operators for Hypergraphs

Fazeny, Ariane *(FAU Erlangen-Nürnberg, Germany)*
Tenbrinck, Daniel *(FAU Erlangen-Nürnberg, Germany)*
Burger, Martin *(FAU Erlangen-Nürnberg, Germany)* 09:10

Traditional graphs are a versatile tool to model relationships in data and can therefore be applied to image processing, machine learning, or other mathematical problems. Hypergraphs are a natural extension of traditional graphs, which also capture higher-order relationships between a group of data entities instead of only allowing pairwise connections. With our work we aim at introducing generalized differential operators on hypergraphs, that are compatible with both the traditional graph case as well as already proposed hypergraph differential operator definitions from the literature. In contrast to previously discussed hypergraph (p-)Laplacians, our definitions induce a trivial first eigenfunction and thus more interpretable

second eigenfunctions. We investigate the potential of the proposed family of hypergraph operators for applications in social network modeling, image processing, and clustering.

S22: Scientific computing

Organizer(s): **Richter, Thomas** *(OVGU Magdeburg)*
Breiten, Tobias *(TU Berlin)*

S22-01: Scientific computing

Date: May 30, 2023 13:30-16:10
Room: HSZ/103

Optimized routes for ship in-ice navigation based on sea ice classifications and ice drift forecasts

Schmitz, Bernhard *(WG Optimisation and Optimal Control, Center for Industrial Mathematics, University of Bremen, Germany; Drift+Noise Polar Services, Bremen, Germany)*
Eis, Christine *(WG Optimisation and Optimal Control, Center for Industrial Mathematics, University of Bremen, Germany)*
Büskens, Christof *(WG Optimisation and Optimal Control, Center for Industrial Mathematics, University of Bremen, Germany)*

13:30

Sea ice retreat as a consequence of climate change leads to increasing shipping activities within polar waters, as newly opened shipping routes can be much shorter than the established ones. Cargo ships benefit from about 30% reduced travel distances between Europe and Asia by taking Arctic passages. Consequently, the demand for time and fuel is strongly reduced. However, navigation in polar waters is still challenging and even dangerous, e.g. because of fast changing ice conditions or unknown bathymetry. Even with having access to proper earth observation data like radar images, ice classifications, or ice charts, manoeuvring in polar waters is not trivial and requires trained staff as well as expert knowledge.

To provide navigational assistance in polar regions, we develop a system that provides route suggestions based on earth observation data, given ship characteristics, bathymetry, and drift / weather models. Using these models, ice classifications derived from earth observation data are interpolated in time to gain high-resolution knowledge about the changing ice conditions.

The resulting 3-dimensional route optimization problem can be solved using an A* algorithm. However, this algorithm is inefficient when applied to long-distance routes, as large datasets offer too many possible combinations of connecting waypoint candidates. To overcome this issue, different methods are tested, which can be divided in two categories: preprocessing steps and further modification of the A* algorithm. The preprocessing techniques reduce the number of waypoint candidates, while keeping important information about small features in the ice, like (open) leads or divergence zones. The reduced set of identified waypoint candidates and the connections between them is called 'road map' and serves as input for the A* algorithm. Investigated variants of the A* algorithm include e.g. weighting methods and anytime implementations. Both approaches and their combination are evaluated in terms of efficiency and reasonability.

A nonconforming finite element method to solve viscous-plastic flow problems on the sphere

Mehlmann, Carolin *(Otto-von-Guericke Universität, Germany)* 13:50

Subject of this talk are the mathematical challenges and the numerical treatment of a flow problem with a strongly nonlinear viscous-plastic material law. The considered viscous-plastic (VP) sea ice momentum equation describes the drift of sea ice and is the currently the most used approach in climate modeling. The efficient simulation of cracks in the sea ice cover with the VP sea ice model is still a big challenge.

In this talk, we analyze the structure of the VP momentum equation. Based on the analysis we present a new approach to discretize this viscous-plastic rheology on the on the surface of the sphere. Our numerical approach is based on the nonconforming Crouzeix-Raviart finite element. The Crouzeix-Raviart element implements a discretization of the viscous-plastic stress tensor that suffers from unacceptable small scale noise in the velocity field. To resolve this issue we introduce an edge-based stabilization of the Crouzeix-Raviart element. Through a blend of theoretical considerations and numerical experiments we show that the stabilized non-conforming finite element provides a stable discretization on the sphere.

A Rigorous Mathematical Definition of Particle Methods and its Application in Scientific Computing

Pahlke, Johannes *(MPI-CBG, Germany)* 14:10

Particle methods are a widely used class of algorithms applied in scientific computing to solve complex problems in various fields, such as fluid dynamics, plasma physics, or granular flows. Particle Methods include diverse simulation algorithms, including Discrete Element Methods (DEM), Molecular Dynamics (MD), Reproducing Kernel Particle Methods (RKPM), Particle Strength Exchange (PSE), and Smoothed Particle Hydrodynamics (SPH). Despite the increasing use of particle methods driven by improved computing performance, the relation between these algorithms remains formally unclear, and a unifying formal definition of particle methods is lacking. In our talk, we will present for the first time a rigorous mathematical definition of particle methods. We will demonstrate its importance by applying it to canonical and non-canonical particle algorithms. Further, we demonstrate how our definition can be utilized to prove the application-independent parallelizability of particle methods. Finally, we show how our definition can be used as a basis for designing scientific computing software. We anticipate that our formal definition facilitates the solution of complex computational problems and the implementation of understandable and maintainable software frameworks for scientific computing.

Application of a multirate method to model the degradation of the Iridium Anode Catalyst Layer in a Proton Exchange Membrane Water Electrolyzer

Chang Dominguez, Dayron *(Otto-von-Guericke-Universität, Germany)* 14:30
Dam, An Phuc *(Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg)*
Richter, Thomas *(Otto-von-Guericke-Universität, Germany)*
Sundmacher, Kai *(Max Planck Institute for Dynamics of Complex Technical Systems Magdeburg)*

Hydrogen becomes every day a more suitable choice for using renewable and green sources of energy. Producing it in safe and efficient ways is a desirable goal. One way to produce Hydrogen is a Proton Exchange Membrane Water Electrolyser. However, non-desirable effects like the corrosion of the anodic Iridium base catalyst layer become a severe problem specially under reduced noble metal loading conditions and their mechanisms are still not well understood. The topic of this talk addresses this problem by mathematically modelling the electrochemical processes that take place, applying an efficient solver to it and fitting the parameters to experimental data.

A new model is presented which is focused on the corrosion of the Anode Catalyst Layer and the influence of Hydrogen in this process. It takes into account the microkinetics and the balances of Oxygen and Hydrogen occurring inside the anodic side as a system of ordinary differential equations, and the effect of the permeation of Hydrogen from the cathode side as a transient diffusion problem.

Because of the temporal characteristics of the problem it could be divided into processes that occur *fast* with a certain local periodicity associated and the degradation itself which happens *slowly*. That is why a multirate numerical method published by Frei and Richter in 2020 is proposed to take advantage of this structure and efficiently compute the solutions for long periods of time. Thus, the complexity of the problem is being drastically reduced. The computing time, which is about 17 hours for the fully resolved simulation, gets down to just minutes for the multirate approach.

Finally, we will present the fitting of two different profiles of the experimental data provided by Alia 2019. A parallelized version of simulating annealing method was applied for the fitting purpose. The fit shows that the model is capable of explaining the nonlinear tendency of different degradation profiles for the same parametrization.

Coupled-model implementation and analysis of hydrogen tracking in natural gas pipelines

Benner, Peter *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)* 14:50
Grundel, Sara *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Nayak, Ashwin Sadanand *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*

Integrating 'green hydrogen' generated from renewable sources into already existing natural gas delivery network has been touted as a feasible solution towards reducing greenhouse emissions. Designing and monitoring such pipeline networks require an in-depth study of

the flow dynamics of gas mixtures under uncertain demands and flexible supply situations. Towards this objective, this study focuses on simulating gas quality across the network for variable supply and demand conditions.
The coupled dynamics of flow and mixture transport are tackled separately. A transient non-linear model in the form of auxiliary Euler equations is used to capture the flow dynamics and is subsequently coupled to a transport equation for tracking the components [1]. The solution utilizes the finite element discretization in each pipe linked algebraically at the network nodes. We discuss the particular assumptions and challenges in its implementation. With this regard, a software tool is developed addressing network scalability and model versatility. The tool is aimed to be flexibile providing abstract components for easier integration and also extensible for the various design choices involved in pipeline networks for transporting gas mixtures. A case study is demonstrated with our approach on a large-scale gas network with various supply conditions and compared with available open-source tools [2]. Finally, strategies are discussed towards implementing model reduction methods for the system.

[1] Bermudez., A., Shabani, M., Numerical simulation of gas composition tracking in a gas transportation network, *Energy* (2022)*,* ***247****:123459.*
[2] Himpe C., Grundel, S., Benner, P., Model Order Reduction for Gas and Energy Networks, *J. Math. Ind.* (2021) **11**:13.

A Discontinuous Galerkin Approach for Cloudy Air with Implicit Condensation

Hittmeir, Sabine *(University of Vienna, Austria)*
Lederer, Philip L. *(TU Wien, Austria)*
Schöberl, Joachim *(TU Wien, Austria)*
von Wahl, Henry *(University of Vienna, Austria)*

15:10

Precipitation still causes one of the most significant uncertainties in weather forecasting and climate models. While the equations of dry air are generally accepted, the equations governing cloudy air are still actively debated. Therefore, the numerical simulation of cloudy air models is a critical tool to help investigate the importance of individual thermodynamic components. The equations governing air with warm rain are a set of coupled non-linear transport equations with additional algebraic constraints. They consist of the compressible Euler equations with multiple densities modelling different phases of water, source terms modelling phase-changes. To avoid the difficult modelling of a source term describing phase changes due to condensation, we combine the water phases of water vapour and cloud water into a single density. To recover the vapour density, cloud density and temperature under the constraint of water vapour saturation, a non-linear algebraic problem needs to be solved. We formulate the equations as a hyperbolic conservation law to apply a discontinuous Galerkin (DG) discretisation to solve the system of equations. The DG Explicit time-stepping allows efficient use of high-performance computing hardware through matrix-free routines. This is necessary to solve the huge systems resulting from the large domains of interest. To recover all quantities necessary for the next explicit time step, we solve the algebraic problem point-wise, which also utilises the parallel hardware well. We illustrate the potential of this

approach using numerical examples based on several established problems. This includes higher-order convergence for the case of smooth solutions.

S22-02: Scientific computing

Date: May 31, 2023 08:30-09:30
Room: HSZ/401

Dimensional Reduction for Parametric Projection-based Reduced Order Models in Crash

Lesjak, Mathias *(BMW AG, Germany; School of Engineering and Design, Technical University of Munich, Germany)* 08:30
Duddeck, Fabian *(School of Engineering and Design, Technical University of Munich, Germany)*

Modern car development regarding passive safety strongly relies on finite element simulations. These simulations provide accurate results, however, only in an idealized scenario and just for one point in the parameter space. Robustness and uncertainty studies help to better understand the model as they investigate the behavior of the considered model around this point. This avoids costly revisions at a later point in the design process when the hardware tests, involving many deviations from the idealized simulations, are performed. Due to the immense computational costs, multi-query analysis like robustness studies, optimization and uncertainty quantification are currently not feasible for large simulation models. Reduced order modeling uses already generated data to accelerate future simulations. It relies on the fact, that the dimensions in the data are not independent of each other. Instead, using a data-driven method, a low-rank structure can be identified. The generated mapping is subsequently used to simplify existing models or to generate new models working on the low-dimensional data (non-intrusive models). Projection-based model order reduction (MOR) plays an important role in passive safety, as it is physics-based and has no black-box character as classical machine learning (ML) models. The accuracy of the reduced order model (ROM) heavily relies on the dimensional reduction. Proper orthogonal decomposition (POD) is commonly used to create it. However, this linear method is not able to find a low-dimensional mapping if the variance in the training data is too large, which is typically the case for data generated by highly nonlinear parametric models. As effective hyperreduction depends on a low-dimensional mapping, further methods have to be developed to ensure low dimensionality while maintaining high accuracy. We provide an overview of different strategies for parametric MOR in the context of highly nonlinear solid dynamics like encountered in crashworthiness, discussing potential benefits and drawbacks. We show a successful application of the local reduced order bases approach to a crash problem and present first results using nonlinear dimensional reduction using an autoencoder in this context. Implementation details are given as the co-simulation between a Fortran program and Python is nontrivial. Our work shows the successful application of parametric MOR for crash problems and depicts future research directions.

Block-structured mesh generation from implicit geometries for cardiovascular applications

Bosnjak, Domagoj *(Institute of Structural Analysis, Graz University of Technology, Austria)* 08:50
Fries, Thomas-Peter *(Institute of Structural Analysis, Graz University of Technology, Austria)*

Structured hexahedral mesh generation may be performed via block structures [1], an approach consisting of partitioning the domain into coarse-scale blocks, thereby generating a structure whose topology emulates the domain topology. From there on, each block may be individually meshed to obtain the final domain discretization. However, the generation of the block structure itself is often a cumbersome or even manual task, especially for non-trivial domains.

We present an approach to generating block structures for cardiovascular applications with the help of implicit domain representations. The surface of the domain is described either by a triangulated surface mesh (STL format) from which we obtain a signed distance function, or a convolution surface [2]. In either case, the surface is represented by a single level set function. Alongside this, we also compute the skeleton [3], i.e. the centerline of the domain. Since the focus is on cardiovascular applications, we seek to mesh blood vessels, both healthy and pathological. As significant topological differences between different domains are possible, e.g., the number of connected (smaller) blood vessels in the case of an aorta, it is important to point out that the skeleton-based implicit approach does not suffer from topology-dependence, thus no domain templates are required. Instead, prototypes for generating blocks are provided based on the different configurations in the skeleton. The surface points of the block structure are aligned to the surface of the domain via closest point projection, or Newton iterations, depending on the choice of the surface representation. Finally, the mesh is obtained via transfinite maps, from the topology information given by the block structure and the geometry information given by the level set function representing the surface.

[1] Ali Z., Tyacke J., Tucker P.G., Shahpar S.: Block Topology Generation for Structured Multi-block Meshing with Hierarchical Geometry Handling, Procedia Engineering, 163, 212-224, 2016

[2] Fuentes Suarez A. J., Hubert E., Zanni C.: Anisotropic convolution surfaces, Computers & Graphics, 82, 106-116, 2019

[3] Au O., Tai C.-L., Chu H-K., Cohen-Or D., Lee T.-Y.: Skeleton Extraction by Mesh Contraction. ACM Transactions on Graphics, 2008

S22-03: Scientific computing

Date: May 31, 2023 14:00-16:00
Room: HSZ/103

Can neural networks replace traditional numerical methods for partial differential equations?

Lessig, Christian *(Otto-von-Guericke-Universität Magdeburg, Germany)* 14:00

Deep neural networks have led to tremendous progress in the past 15 years, for example in computer vision and natural language processing. For the solution of partial differential equations, different neural network-based approaches have also been explored. Most current results are, however, far from practical and lack behind the progress that neural networks have provided in other areas. In this talk, I will highlight some examples where deep neural networks already outperform traditional solvers for two- and three-dimensional flow problems of practical importance. Based on these, I will discuss why, in my opinion, progress was possible for these problems and has not been achieved elsewhere. Some conclusions will be drawn on what can advance neural network-based methods for partial differential equations in general in the next years and what contribution a mathematical analysis of the methods can provide. It will also be discussed which role large scale representation learning, which is the methodology behind large language models such as GPT-3 and PaLM, can play in scientific computing and for numerical methods for partial differential equations (beyond writing papers).

Benchmarking Hybrid Finite Element/Deep Neural Networks and Classical Finite Element Methods in 2D and 3D

Margenberg, Nils *(Helmut Schmidt University Hamburg, Germany)*
Jendersie, Robert *(Otto von Guericke University Magdeburg, Germany)*
Anselmann, Mathias *(Helmut Schmidt University Hamburg, Germany)*
Bause, Markus *(Helmut Schmidt University Hamburg, Germany)*
Lessig, Christian *(Otto von Guericke University Magdeburg, Germany)*
Richter, Thomas *(Otto von Guericke University Magdeburg, Germany)* 14:40

Accurate flow simulations remain a challenging task. Combining classical finite element approximation techniques with deep neural neworks adds new aspects to the pure numerics-oriented approach and offers potential for further innovations. In this talk we discuss the use of deep neural networks for augmenting classical finite element simulations in fluid-dynamics. First, we establish new benchmark results for the classical DFG-benchmarks in 2D and 3D with high accuracy. We extend these settings to higher Reynolds numbers and compare two implementations based on the FEM libraries Gascoigne3D and deal.II. This implies the choice of two different approaches for the discretization: In Gascoigne3D we use equal-order elements in space with local projection stabilization and a Crank-Nicholson time stepping scheme. In deal.ii we use a space-time finite element discretization of higher-order: In space we use inf-sup stable pairs and discontinuous Galerkin methods in time. A comparison of the computation of drag and lift forces across the two software platforms in 2D and

3D benchmark settings show that they are in good agreement. At high Reynolds numbers, accurate simulations especially in 3D become increasingly difficult and the classical methods reach their limits. Although the finite element method is highly efficient and established for the discretization of the Navier-Stokes equations, fundamental problems, such as the resolution of fine structures or a correct information transport between scales, are still not sufficiently solved. We discuss approaches to connect the finite element method with neural networks to overcome these limitations. The paradigm is to use classical simulation techniques when their strengths are eminent, such as in the efficient representation of a coarse, large-scale flow field. Neural networks are used when a full resolution of the effects does not seem possible or efficient. Inspired by these ideas, the Deep Neural Network Multigrid Solver combines a geometric multigrid solver and a deep neural network. We show the efficiency, generalizability and scalability by 2D and 3D simulations. In addition to the desired increase in efficiency, the focus is particularly on issues of stability, generalizability and error accuracy. The error accuracy is established by comparison of the Deep Neural Network Multigrid Solver with the newly established benchmark results.

Domain Decomposition with Neural Network Interface Approximations for time-harmonic Maxwell's equations with different wave numbers

Knoke, Tobias *(Leibniz University Hannover, Germany)*
Kinnewig, Sebastian *(Leibniz University Hannover, Germany)*
Beuchler, Sven *(Leibniz University Hannover, Germany)*
Demircan, Ayhan *(Leibniz University Hannover, Germany)*
Morgner, Uwe *(Leibniz University Hannover, Germany)*
Wick, Thomas *(Leibniz University Hannover, Germany)*

15:00

In this talk, we consider the time-harmonic Maxwell's equations and their numerical solution with a domain decomposition method. As an innovative feature, we propose a neural network-enhanced approximation of the interface conditions between the subdomains. To substantiate this proof of concept, we investigate a few subdomains in some numerical experiments with low frequencies. Moreover, we highlight current challenges of training and testing with different wave numbers and we provide information on the behaviour of the neural-network, such as convergence of the loss function, and different activation functions.

Analysis of a hybrid finite element / neural network solver

Kapustsin, Uladzislau *(Otto-von-Guericke-Universität Magdeburg, Germany)*
Richter, Thomas *(Otto-von-Guericke-Universität Magdeburg, Germany)*
Kaya, Utku *(Otto-von-Guericke-Universität Magdeburg, Germany)*

15:20

Obtaining a solution of a partial differential equation (PDE) is one of the central problems of numerical analysis. PDEs frequently arise in engineering and science, thus efficient methods for solving them are highly demanded. Due to that, there are many well-established methods, e.g. the Finite Element Method. On the other hand, the ongoing rise of machine learning has led to many attempts to also apply it to various mathematical problems, including solving a PDE. Some approaches, like Physics-Inspired Neural Networks (PINNs), rely on conversion of the PDE into an optimization problem. These approaches perform well when applied to some

particular classes of problems, but in general they do not offer many advantages over classical methods. Another problem with PINNs is a need to retrain a neural network when a problem changes. There are other methods that tackle this problem, but they still have another one, which is a lack of mathematical guarantees for the resulting solution. In this talk an alternative approach will be presented which is a combination of the Finite Element Method and machine learning techniques. The proposed method uses neural networks not to solve a PDE directly, but rather to refine an already existing coarse finite element solution, which distinguishes it from the aforementioned methods. The proposed method starts by considering a set of PDEs, which will be further used as a training set. In particular, for training it is necessary to obtain coarse and fine solution for each of those training problems. After that, one can apply the network to the coarse solution in order to obtain a network solution. Then the error between the resulting solutions and corresponding fine solutions is computed and used to fit the parameters of the neural network. Once the network is trained, it can be applied to the problems not belonging to the original training set, thus eliminating the necessity to retrain. It's also very important to note that the proposed method operates locally. The proposed method works by first subdividing the domain of the problem into a set of subdomains. Then a neural network is being applied locally, i.e. to the coarse solution restricted to each of those subdomains. Afterwards, those refined local solutions are combined into a new global solution, which is an improvement over the coarse solution that we started with. Preliminary results on stability of the proposed method will also be presented.

Parameter Identification of Piezoelectrics improved by Neural Networks

Jurgelucks, Benjamin *(Zuse Institut Berlin / Humboldt-Universität zu Berlin, Germany)* 15:40

Accurately determining material parameters of piezoelectric materials is a demanding undertaking as some material parameters express only low sensitivity and are thus very hard to reconstruct as part of an inverse problem using classical methods alone. In recent years many advances have been made on this topic such as increasing the sensitivity of low-sensitivity parameters via optimal design of experiments and providing accurate and cheap gradient information via Algorithmic Differentiation. However, as classical gradient-based optimization methods for inverse problems only converge locally providing an accurate initial guess of the parameters is particularly important.

Because of the curse of dimensionality using machine learning techniques to accurately determine the material parameters requires a huge amount of data und thus solutions to the governing partial differential equation. However, by only requiring approximately correct parameter values less data is needed. These approximately correct parameter values can instead be provided to classical methods for inverse problems as the initial guess. This greatly enhances the variety of different piezoelectric materials of which material parameters can now be identified.

S22-04: Scientific computing

Date: June 1, 2023 08:30-10:30
Room: HSZ/103

Computational Approaches to H-infinity-robust Controller Design for Large-scale Systems

Heiland, Jan *(Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg, Germany; Otto-von-Guericke-Universität Magdeburg, Germany)*
Benner, Peter *(Max-Planck-Institut für Dynamik komplexer technischer Systeme, Magdeburg, Germany; Otto-von-Guericke-Universität Magdeburg, Germany)*
Werner, Steffen W.R. *(NYU Courant Institute of Mathematical Sciences, New York, USA)*

08:30

The computation of controller gains for the (linearization based) H_∞ robust control of linear (and nonlinear) dynamical systems amounts to the solution of indefinite Riccati equations. For large-scale systems, a direct approach is infeasible because of both computational efforts and memory requirements. In this talk we review existing iterative approaches and then discuss our recent algorithm[1] that merges the ideas of the *Riccati iteration*[2] (that approaches solutions of the indefinite equations through a sequence of definite Riccati equations) and *low-rank ADI iterations*[3] (as it has become a standard tool for solving large-scale Riccati equations numerically). For that we provide necessary and sufficient conditions for convergence and thorough numerical studies concerning run times and memory consumption. In order to estimate the performance and robustness of controllers, one may resort to system norms which themselves pose a significant computational challenge. In the second part of this talk, we will illustrate suitable reformulations of the relevant system norms so that their estimation can be achieved by high-performant routines from numerical linear algebra[4]. In view of robust control, we will in particular focus on estimates that also include system uncertainties and model reduction errors. Finally, we will bring together the computation of the controller gains and the norm estimates to robustly stabilize incompressible flows in two different setups of the well-known cylinder wake.

[1] Benner, P.; Heiland, J. & Werner, S. W. R. *A low-rank solution method for Riccati equations with indefinite quadratic terms*, Numer. Algorithms, 2022.
[2] Lanzon, A.; Feng, Y. & Anderson, B.: *An iterative algorithm to solve Algebraic Riccati Equations with an indefinite quadratic term*, 2007 European Control Conference (ECC), 2007.
[3] Benner, P.; Bujanović, Z.; Kürschner, P. & Saak, J.: *RADI: A low-rank ADI-type algorithm for large scale algebraic Riccati equations*. Numer. Math., 2018.
[4] Benner, P.; Heiland, J. & Werner, S. W. R.: *Robust output-feedback stabilization for incompressible flows using low-dimensional H_∞-controllers*. Comput. Optim. Appl., 2022, 82, 225-249.

Approximation of the uncertainty propagation of initial value perturbations in coupled thermal models

Naumann, Andreas *(TU Chemnitz, Germany)* 09:10
Herzog, Roland *(Heidelberg University, Germany)*

Recent development and operation of machine tools demand for increasing accuracy. Numerical simulations are an indispensable tool for the accurate prediction of the temperature field. This prediction depends strongly on the certainty of the model parameters, which include especially the initial conditions. Due to the size of machine tools, the initial temperatures cannot be measured in all points. Therefore the temperature field must be, at least partially, inferred from measurements and a model.

We consider the thermal finite element model of a tool machine, equipped with temperature sensors. We derive the posterior variance of the initial temperature and compare some numerical methods to approximate the posterior variance.

Parallelization in time for optimal control and inverse problems

Götschel, Sebastian *(Hamburg University of Technology, Germany)* 09:30

Large-scale optimization problems governed by time-dependent partial differential equations (PDEs) occur in a multitude of applications, for example in inverse problems for non-destructive testing of materials and structures, or in optimal control problems related to individualized medicine. Algorithms for the numerical solution of such PDE-constrained optimization problems are computationally extremely demanding, as they require multiple PDE solves during the iterative optimization process. With today's modern computers, the time-to-solution can be decreased through massive parallelization, which is traditionally done in the spatial dimensions. In addition, time-parallel methods have received increasing interest in recent years to overcome scaling limits. In this talk, we investigate approaches to use parallel-in-time methods for the solution of PDE-constrained optimization problems, and present numerical examples.

A Dynamic Bayesian Network Approach for Digital Twins

Henning, Julian *(Universität Ulm; ATR Software GmbH)* 09:50
Urban, Karsten *(Universität Ulm)*

Until now, there is no universally accepted definition of the term "Digital Twin". Nonetheless, all definitions of a Digital Twin encapsulate the idea that a physical entity is replicated in a digital model and that there exists some kind of interaction between the physical and the Digital Twin. Typically, data from the real entity is captured and used to improve the quality of the digital model. The Digital Twin, on the other hand, is used to make predictions about the future which influence the control of the physical twin. A particular promising field of application is manufacturing, particularly production lines. Here, Digital Twins can be used to predict machine failures (which enables predictive maintenance) and the quality of products (also known as predictive quality). However, this application is also challenging, because there exist numerous interactions between products and machines: The state of one or multiple machines influence the state of one or multiple products and vice versa. These

interactions can be modeled with Dynamic Bayesian Networks. Individual physical or chemical processes or entities which occur inside the system, on the other hand, can be model with Parametrized Partial Differential Equations (PPDEs). These partial differential equations need to be constantly solved throughout the life cycle of the real entity. Therefore, we are in a multi-query setting. Furthermore, the solving of the partial differential equations should, ideally, be possible in real time. Model Order Reduction (MOR) can be used to tackle both issues by building reduced models. In this talk, we want to describe an approach for using Digital Twins based on Dynamic Bayesian Networks. These utilize reduced order models as well as machine learning approaches to maintain a close approximation of the actual state of a system and to make predictions about the future. The approach is based on the work by Karen E. Willcox [1], but extends the original approach by an interaction component between multiple Digital Twins. This work is part of the research project "Digitale Prüfplattform für die Fahrzeug- und Zuliefererindustrie (DigiPrüf)", which is funded by the "Bundesministerium für Wirtschaft und Klimaschutz der Bundesrepublik Deutschland" under the "Konjukturpaket 35c Modul a2".

[1] M. G. Kapteyn, D. J. Knezevic, and K. Willcox. Toward predictive digital twins via component-based reduced-order models and interpretable machine learning. AIAA Scitech 2020 Forum, 2020.

Adjacency-based, non-intrusive reduced-order modeling for Fluid-Structure Interactions

Gkimisis, Leonidas *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Richter, Thomas *(Otto-von-Guericke-Universität Magdeburg, Germany)*
Benner, Peter *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany; Otto-von-Guericke-Universität Magdeburg, Germany)*

10:10

Non-intrusive model reduction has been developed to become a promising solution to system dynamics forecasting, especially in cases where data are collected from experimental campaigns or proprietary software simulations. In this work, we present a method for non-intrusive model reduction applied to fluid-structure interaction problems. The approach is based on the a priori known sparsity of the full-order system operators (e.g. of the discretized Navier-Stokes equations), which is dictated by grid adjacency information. In order to enforce this type of sparsity, we solve a "local", regularized least-squares problem for each degree of freedom on a grid, considering only the training data from adjacent nodes, thus making computation and storage of the inferred full-order operators feasible. After constructing the non-intrusive, sparse full-order model, the Proper Orthogonal Decomposition is used for its projection to a reduced dimension subspace and thus the construction of a reduced-order model (ROM). This approach differs from methods where data are first projected to a low-dimensional manifold, since here the inference problem is solved for the original, full-order system, assuming sparsity. The methodology is applied to the challenging Hron-Turek benchmark FSI3, for Re = 200. A data-driven, non-intrusive ROM is constructed to predict the two-way coupled dynamics of a solid with a deformable, slender tail, subject to an incompressible, laminar flow. Results considering the accuracy and predictive capabilities of the inferred reduced models are analytically discussed.

S22-05: Scientific computing

Date: June 2, 2023 08:30-10:30
Room: HSZ/103

Diagonally Addressed Matrix Nicknack: Sparse Matrix Vector Product

Saak, Jens *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*
Schulze, Jonas *(Max Planck Institute for Dynamics of Complex Technical Systems, Germany)*

08:30

We suggest a technique to reduce the storage size of sparse matrices at no loss of information, which exploits the typically low matrix bandwidth of matrices arising in applications. We call our technique Diagonally-Addressed (DA) storage. For memory-bound algorithms, a reduction in traffic has direct benefits for both classical (fixed-precision) and multi-precision algorithms. In particular, we demonstrate how to apply DA storage to the Compressed Sparse Rows (CSR) format and compare the performance in computing the Sparse Matrix Vector (SpMV) product, which is a basic building block of many iterative algorithms in scientific computing. We observe a single-threaded performance uplift of up to 15% of 16-bit indices over 32-bit ones, when the traffic exceeds the size of the last-level CPU cache. Ongoing efforts are concerned with multi-threading and vectorization.

Discrete Event Estimation for Spectral Deferred Corrections

Bolten, Matthias *(Bergische Universität Wuppertal, Germany)*
Speck, Robert *(Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH, Germany)*
Strake, Julius *(Institute of Energy and Climate Research: IEK-10, Forschungszentrum Jülich GmbH, Germany)*
Wimmer, Lisa *(Bergische Universität Wuppertal, Germany)*
Zhang, Junjie *(Institute of Energy and Climate Research: IEK-10, Forschungszentrum Jülich GmbH, Germany)*

08:50

In order to have a better control and overview of the dynamics of an energy network, an accurate simulation is mandatory. Since modern power systems are more and more complex, simulation techniques have to become more sophisticated. Converters in a power system use high frequency switching to react in every change of the power supply, and simulating this requires a relatively small time step to resolve this behavior. There are already techniques to take switching behavior with repeating, predictable patterns into account, for example approximating a pulse-width modulation (PWM) signal with a sinusoidal wave. In a power system there are also components whose switching behavior depends on the dynamics itself.
In this presentation, the switch estimator applied to the method of spectral deferred corrections (SDC) is presented together with examples to show its performance. After few iterations the switch estimator predicts the time point of the discrete event using interpolation and root finding techniques, and the time step is adapted. After restarting SDC with the new time step the method is able to resolve the singularity more accurate.

Scalability of a HPC framework for mortar based contact problems

Steimer, Christopher *(Universität der Bundeswehr München, Germany)*
Mayr, Matthias *(Universität der Bundeswehr München, Germany; Data Science & Computing Lab, Universität der Bundeswehr München, Germany)*
Popp, Alexander *(Universität der Bundeswehr München, Germany)*
09:10

For some time, mortar methods have been the preferred modeling approach for surface-coupled problems with non-matching grids, as they provide high accuracy and variational consistency. The considerable additional numerical effort introduced by the evaluation of the mortar integrals (especially in three dimensions) requires an efficient and parallelizable framework, that scales well on parallel hardware architectures and is, thus, suitable for the solution of high-fidelity models with potentially several million degrees of freedom. Although mortar methods have been particularly popular in contact mechanics (among other multi-physics problems), the efficiency of the computations has only recently been targeted and many opportunities for improvement remain.

It has recently been shown that aggregation based algebraic multigrid (AMG) methods can be used as highly efficient and scalable preconditioners for mortar-based contact problems in saddle-point formulation [2]. Furthermore, dynamic load balancing of core kernels, as proposed in [1], allows for a parallel evaluation of mortar operators and their linearizations.

This contribution discusses recent findings on the combined application of AMG and dynamic load balancing techniques to mortar based, large deformation contact formulations. Although weak [1, 2] and strong scaling [1] has been proven for the methods individually, the scalability of the interplay of AMG and dynamic load balancing has yet to be studied and will be presented. Additionally, the reduced impact of the HPC framework on the overall time to solution will be showcased by a high fidelity contact simulation.

References

[1] Matthias Mayr and Alexander Popp. Scalable computational kernels for mortar finite element methods. *Engineering with Computers*, jan 2023.

[2] Tobias A. Wiesner, Matthias Mayr, Alexander Popp, Michael W. Gee, Wolfgang A. Wall. Algebraic multigrid methods for saddle point systems arising from mortar contact formulations. *IJNME, 122(15):3749-3779,2021*.

The numerical flow iteration for the Vlasov equation

Wilhelm, Rostislav-Paul *(RWTH Aachen, Germany)*
Kirchhart, Matthias *(RWTH Aachen, Germany)*
09:30

The Vlasov equation is a high-dimensional partial differential equation arising from kinetic theory and used to model the behaviour of plasma flows in collision-less and strongly non-equilibrium regimes. The six-dimensional phase-space and the turbulent motion of plasmas together with formation of strong filamentation in the solution lead to significant complications for numerical solvers: Solvers based on a phase-space grid offer good accuracy, but they suffer from extensive memory-usage due to storage as well as management of the high-dimensional grid. Furthermore the inherent numerical diffusion and restrictive CFL conditions lead to loss of conservation properties as well as long run-times. The alternatively used Lagrangian schemes, like Particle-In-Cell, can overcome these problems to a certain extend,

however, the inherent numerical noise reduces the quality of the obtained solution. We present a novel approach, the numerical flow iteration (NuFI), which evaluates the numerical solution via storing the three-dimensional electric potentials, using these to iteratively reconstruct the Lagrangian flow and directly evaluating the initial data via the method of characteristics. This reduces the total memory-requirement by several orders of magnitude and allows to shift workload from frequent memory access to computations on the fly, i.e., yielding high flop/Byte-rates, which is favourable on modern compute-architectures. Furthermore using the Lagrangian formulation one conserves desired properties like L^p-norms and kinetic entropy exactly, as well as total energy up to time-integration error. We demonstrate the accuracy and scalability of the new approach on several test-cases in up to six dimensions showing computations done on a local workstation as well as a GPU-cluster.

Viscoelastic model hierarchy for the simulation of fiber melt spinning of semi-crystalline polymers including radial effects

Ettmüller, Manuel *(Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany)* 09:50
Arne, Walter *(Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany)*
Marheineke, Nicole *(Universität Trier, Lehrstuhl Modellierung und Numerik, Trier, Germany)*
Wegener, Raimund *(Fraunhofer Institute for Industrial Mathematics ITWM, Kaiserslautern, Germany)*

Fiber melt spinning plays an important role in the production of polymer materials. In the case of semi-crystalline polymers, crystallization occurs during the melt spinning process, which has a significant impact on the properties of the final product. Experiments have shown that the degree of crystallization is not homogenous over the cross-section of the fiber. For modeling and simulation, this means that the otherwise usual cross-sectional averaging of all fiber quantities does not cover all relevant phenomena. This opens up the question which model equations need to be resolved in radial direction and which can be cross-sectionally averaged. For this purpose, we present a hierarchy of viscoelastic fiber models ranging from a complex, fully resolved three-dimensional model to a completely cross-sectionally averaged model. Simulation results of all models within the hiearchy are then analyzed with respect to accuracy and efficiency.

S22-06: Scientific computing

Date: June 2, 2023 11:00-13:00
Room: HSZ/103

A mechanically consistent model for fluid-structure interactions with contact including seepage

Frei, Stefan *(University of Konstanz, Germany)* 11:00
Burman, Erik *(University of Konstanz, Germany)*
Fernández, Miguel Angel *(University of Konstanz, Germany)*

We present a new approach for a mechanically consistent modelling and simulation of fluid-structure interactions (FSI) with contact. The fundamental idea consists of combining a relaxation of the contact conditions with the modelling of seepage through a porous layer of co-dimension one during contact. For the latter, a Darcy model is considered in a thin porous layer attached to a solid boundary in the limit of infinitesimal thickness. The resulting computational model is both mechanically consistent and simple to implement. The FSI coupling and the contact conditions are imposed weakly by means of a unified Nitsche approach. We analyse the approach in detailed numerical studies with both thick and thin-walled solids, within a fully Eulerian and an immersed approach and using fitted and unfitted finite element discretisations.

A wavelet-enhanced adaptive hierarchical FFT-based approach for the efficient solution of microscale boundary value problems

Kaiser, Tobias *(Technical University of Dortmund, Germany)* 11:20
Raasch, Thorsten *(University of Siegen, Germany)*
Remmers, Joris J. C. *(Eindhoven University of Technology, The Netherlands)*
Geers, Marc G. D. *(Eindhoven University of Technology, The Netherlands)*

We report on an adaptive, hybrid numerical solver for microscale boundary value problems that combines adaptive wavelet methods with FFT techniques. In the classical Moulinec-Suquet scheme, the governing fields are represented in the coordinates of an interpolating wavelet basis, thereby enabling fast local wavelet transforms and adaptive grid refinement. Localized features can be resolved accurately, while the number of evaluations of the material model can be significantly reduced. The results are illustrated by a series of one- and two-dimensional numerical studies.

Adaptive parallel space-time discontinuous Galerkin Methods for the linear transport equation

Wieners, Christian *(KIT, Germany)* 11:40

We consider variational space-time discretizations for the linear transport equation with full upwind discontinuous Galerkin finite elements in space and time. We show that hybridization of the system by introducing face degrees of freedom yields a symmetric positive definite system.

Based on our convergence analysis for symmetric Friedrichs systems in a mesh-dependent DG norm we construct an error estimator and show numerically that the adaptive method is efficient. The linear system is solved by a multigrid method in space and time, and we show

numerically that the convergence is of optimal complexity. We observe that convergence is obtained also in case of discontinuous solutions without regularity requirements.

Finally, we show that in case of local sources and local goal functionals the computational domain can be restricted to a subset of the space-time cylinder and that then a suitable parallel strategy results in a significant reduction of the computational effect.

Efficient simulation of incompressible flows: a parallel finite element algorithm with semi-explicit time integration and local pressure-corrections

Kaya, Utku *(Otto-von-Guericke-University Magdeburg, Germany)*
Richter, Thomas *(Otto-von-Guericke-University Magdeburg, Germany)*
12:00

This talk presents a novel approach for solving the three-dimensional incompressible Navier-Stokes equations using a parallel finite element algorithm. Three key features of the algorithm will be discussed to reduce the computational costs. Firstly, an explicit time stepping scheme for the momentum equation eliminates the need to invert a system matrix. Secondly, the nonlinear term is approximated with a pre-assembled matrix, circumventing the need for spatial integration. Finally, the coupling between velocity and pressure is handled through local pressure-corrections [1], making the parallelization of the pressure-related Poisson equation straightforward. The performance of the algorithm will be demonstrated through numerical experiments, showing its suitability for parallel approximations of complex incompressible flows.

[1] U. Kaya, R. Becker, and M. Braack. Local pressure-correction for the Navier-Stokes equations. *International Journal for Numerical Methods in Fluids*, 93(4):1199–1212, 2021

Matrix-free preconditioners for isogeometric discretization of the Stokes equations

Mika, Michał Łukasz *(Technical University of Darmstadt, Germany)*
Hiemstra, René Rinke *(Technical University of Darmstadt, Germany)*
ten Eikelder, Marco Frederik Petrus *(Technical University of Darmstadt, Germany)*
Schillinger, Dominik *(Technical University of Darmstadt, Germany)*
12:20

Fast formation and assembly techniques on tensor-product spaces have been proven to robustly reduce the computational cost of formation and assembly by orders of magnitude. The application of such techniques in the context of Navier-Stokes, Navier-Stokes-Korteweg, Cahn-Hilliard and similar equations enables high resolution of the underlying physics and thus are of interest for future model and method development. Naturally, leveraging similar techniques and properties in the design of robust preconditioners for iterative solvers is of no lesser importance. In the current work we focus on preconditioning systems arising from Stokes equations discretized by structure-preserving isogeometric Raviart-Thomas spline spaces with weak tangential boundary conditions. Our approach builds upon the state of the art preconditioners based on the Fast Diagonalization method. We propose a preconditioning strategy to further enhance the effectiveness and maintain high efficiency. To address the effectiveness aspect, we discuss the conditioning as well as the spectra of the preconditioned system. The efficiency is addressed by theoretical estimates of the algorithmic complexity of the preconditioner application, which are verified numerically to be $O(N^{3/2})$

in 2D and $O(N^{4/3})$ in 3D, where N is the number of degrees of freedom. The proposed preconditioning strategy is benchmarked against state of the art isogeometric preconditioners for Stokes systems. Our work is accompanied by an open-source Julia implementation of the discussed techniques.

Towards a Benchmark Framework for Model Order Reduction in the Mathematical Research Data Initiative (MaRDI)

Benner, Peter *(Max-Planck-Institut für Dynamik komplexer technischer Systeme)*
Himpe, Christian *(Westfälische Wilhelms-Universität Münster)*
Lund, Kathryn *(Max-Planck-Institut für Dynamik komplexer technischer Systeme)*
Mitchell, Tim *(Max-Planck-Institut für Dynamik komplexer technischer Systeme)*
Saak, Jens *(Max-Planck-Institut für Dynamik komplexer technischer Systeme)*
Stage, Alexander *(Max-Planck-Institut für Dynamik komplexer technischer Systeme)*

12:40

The race for the most efficient, accurate, and universal algorithm in scientific computing drives innovation. At the same time, this healthy competition is only beneficial if the research output is actually comparable to prior results. Fairly comparing algorithms can be a complex endeavor, as the implementation, configuration, compute environment, and test problems need to be well defined. Due to the increase in computer-based experiments, new infrastructure for facilitating the exchange and comparison of new algorithms is also needed. To this end, we propose a benchmark framework, as a set of generic specifications for comparing implementations of algorithms using test problems native to a community. Its value lies in its ability to fairly compare and validate existing methods for new applications, as well as compare newly developed methods with existing ones.

As a prototype for a more general framework, we have begun building a benchmark tool for the Model Order Reduction Wiki (MORWiki). The wiki features three main categories: benchmarks, methods, and software. An editorial board curates submissions and edits entries. Data sets for linear and parametric-linear models are already well represented in the existing collection. Data sets for non-linear or procedural models, for which only evaluation data, rather than equations, are available, are being added and extended. Properties and interesting characteristics used for benchmark selection and later assessments are recorded in the model metadata.

The Model Order Reduction Benchmarker (MORB) is under active development for linear time-invariant systems and solvers. An ontology (MORBO) and knowledge graph are being developed in parallel, which catalogue benchmark problem sets and their metadata and will be integrated into the Mathematical Research Data Initiative (MaRDI) Portal, to help improve the findability of such data sets. MORB faces a number of technical and field-specific challenges, and we hope to recruit community input and feedback while presenting some initial results.

S23: Applied operator theory

Organizer(s): **Chill, Ralph** *(TU Dresden)*
Waurick, Marcus *(TU Freiberg)*

S23-01: Applied operator theory

Date: May 31, 2023 14:00-16:00
Room: HSZ/101

Spectral inclusions and approximations of finite and infinite banded matrices

Lindner, Marko *(TU Hamburg (TUHH), Germany)* 14:00

We derive inclusion sets and approximations to spectrum and pseudospectrum of banded, in general non-normal, matrices of finite or infinite size. In the infinite case (bi- or semi-infinite), the matrix acts as a bounded linear operator on the corresponding l^2 space, and we moreover bound and approximate its essential spectrum.

Our inclusion sets come as unions of pseudospectra of certain submatrices of chosen size. Via this choice, we can balance accuracy against numerical cost. The philosophy is to split one global spectral problem into several local problems of moderate size.

Operator splitting based dynamic iteration for linear infinite-dimensional port-Hamiltonian systems

Farkas, Balint *(Bergische Universität Wuppertal, Germany)* 14:40
Jacob, Birgit *(Bergische Universität Wuppertal, Germany)*
Reis, Timo *(TU Ilmenau, Germany)*
Schmitz, Merlin *(Bergische Universität Wuppertal, Germany)*

A dynamic iteration scheme for linear infinite-dimensional port-Hamiltonian systems is proposed. The dynamic iteration is monotone in the sense that the error is decreasing, it does not require any stability condition and is in particular applicable to port-Hamiltonian formulations arising from domain decompositions.

Infinite-Dimensional Control Systems as Evolutionary Equations

Buchinger, Andreas *(TU Bergakademie Freiberg, Germany)* 15:00

The theory of evolutionary equations respectively evolutionary well-posedness of PDEs - that means unique solvability as well as continuous and causal dependence on given data - is a concept afforded by Rainer Picard et al. In this talk, a possible evolutionary approach to controllability and observability of PDEs and to control theory for PDEs in general is presented.

Weak Observability Estimates for the Heat Equation on Discrete Graphs

Seifert, Christian *(Technische Universität Hamburg, Germany)* 15:20

We consider a weighted discrete graph b over (X,m), i.e. X is a countable discrete set, m is a function on X which induces a measure and b is an edge weight. Then the corresponding Laplacian is a non-negative self-adjoint operator.

We investigate the question of weak observability for the corresponding heat equation, i.e. we study if, for given final time *T>0* and a subset *D* of *X*, the norm of the solution of the heat equation at time *T* can be bounded by the portions of the solution on *D* up to time *T* and the norm of the initial condition.
This is joint work with Peter Stollmann (Chemnitz) and Martin Tautenhahn (Leipzig).

Pathwise Uniform Convergence of Time Discretisation Schemes for SPDEs

Klioba, Katharina *(Technische Universität Hamburg, Germany)* 15:40

In this talk, we showcase results on convergence rates for time discretisation schemes for semi-linear stochastic evolution equations with additive or multiplicative Gaussian noise. The leading operator is assumed to be the generator of a strongly continuous semigroup on a Hilbert space, and the focus is on hyperbolic problems. The main results are optimal bounds for the uniform strong error, which is the p-th moment of the supremum in time of the error for $p \in [2, \infty)$.

The usual schemes such as splitting/exponential Euler, implicit Euler, and Crank-Nicolson, etc. are included as special cases. Under conditions on the nonlinearity and the noise we show that the error decays as $k \cdot log(T/k)$ for the linear equation with additive noise for general semigroups and as $\sqrt{k} \cdot log(T/k)$ for the nonlinear equation with multiplicative noise for contractive semigroups. The logarithmic factor can be removed if the splitting scheme is used with a (quasi)-contractive semigroup. The obtained bounds coincide with the optimal bounds for SDEs.

Most of the existing literature is concerned with bounds for the simpler pointwise strong error, where the supremum in time is taken of the p-th moment of the error and not vice versa. Applications to the Schrödinger equation are discussed, which improve and reprove existing results with a unified method.

This is joint work with Mark Veraar and Jan van Neerven (TU Delft).

S23-02: Applied operator theory

Date: June 2, 2023 11:00-13:00
Room: HSZ/101

Sharp boundary trace theory for second order elliptic operators on Lipschitz domains

Behrndt, Jussi *(TU Graz, Austria)* 11:00

We develop a sharp boundary trace theory in arbitrary bounded Lipschitz domains which, in contrast to classical results, allows "forbidden" endpoints and permits the consideration of functions exhibiting very limited regularity. This is done at the (necessary) expense of stipulating an additional regularity condition involving the action of theelliptic operator on the functions in question which, nonetheless, works perfectly with the Dirichlet and Neumann realizations. In turn, this boundary trace theory serves as a platform for developing a spectral theory for second order partial differential operators on bounded Lipschitz domains, along with their associated Weyl-Titchmarsh operators.

This talk is based on joint work with Fritz Gesztesy and Marius Mitrea.

Quasi Gelfand triple

Skrepek, Nathanael *(TU Freiberg, Germany)* 11:40

We generalize the notion of Gelfand triples (also called Banach- Gelfand triples or rigged Hilbert spaces) by dropping the necessity of a continuous embedding. This means in our setting we lack of a chain inclusion. We replace the continuous embedding by a closed embedding of a dense subspace. This new notion will be called quasi Gelfand triple. These triples appear naturally, when we regard the boundary spaces of spatially multidimensional differential operators, e.g. the Maxwell operator. We will show that there is a smallest space where we can continuously embed the entire triple. Moreover, we show that every quasi Gelfand triple can be decomposed into two "ordinary" Gelfand triples.

G-convergence of Friedrichs systems

Burazin, Krešimir *(University of Osijek, Croatia)*
Erceg, Marko *(Faculty of Science, University of Zagreb, Croatia)*
Waurick, Marcus *(Faculty of Mathematics and Computer Science, TU Bergakademie Freiberg, Germany)* 12:00

The theory of abstract Friedrichs operators, introduced by Ern, Guermond and Caplain (2007), proved to be a successful setting for studying positive symmetric systems of first order partial differential equations (Friedrichs, 1958), nowadays better known as Friedrichs systems. Since Friedrichs systems encompass many standard equations of mathematical physics, irrespective of their type, this provides a framework for developing a unified theory for linear partial differential equations. In this talk we are focused on the problem of homogenisation of Friedrichs systems, i.e. we study a sequence of problems and study the behaviour on the limit. The answer is given in the form of the G-convergence of (a class of) Friedrichs systems

and its represent a refinement and a generalisation of the results given in Burazin, Vrdoljak (2014).

Holomorphic G-convergence

Waurick, Marcus *(TU Bergakademie Freiberg, Germany)* 12:20

G-convergence is a mathematical tool to understand homogenisation processes of sequences of self-adjoint multiplication operators as coefficients in (standard) divergence form problems. It has been found that this type of convergence can be recast into convergence in the weak operator topology of a canonically associated sequence of operators. In the talk we provide an equivalent formulation of this convergence which will eventually enable us to generalise the notion of G-convergence to operator sequences that do not satisfy any coercivity conditions. The more general limit procedure – holomorphic G-convergence – can then be applied to divergence form problems with highly oscialltory sign-changing coefficients. By means of an example we show that the period-to-zero limit of periodic, sign-changing coefficients may lead to a nonlocal, 4th order limit equation, whereas for any strictly positive period the operators considered were local and of 2nd order. The talk is based on `https://arxiv.org/abs/2210.04650`.

Spectral properties of Dirichlet Laplacian in spiral-shaped regions

Exner, Pavel *(Nuclear Physics Institute, Czech Academy of Sciences, Czech Republic)* 12:40

We discuss properties of Dirichlet Laplacian in spiral-shaped regions, in particular, their discrete spectrum. If the spiral is Archimedean, the spectrum is absolutely continuous away from the thresholds and its discrete part is empty; in the asymptotically Archimedean case it may or may not exists, the answer depending on the sign of the next-to-leading term in the asymptotics. If the coil width tends to zero, the spectrum is naturally purely discrete and one can derive a Lieb-Thirring-type inequality for its moments.

S24: History of applied mathematics and mechanics

Organizer(s): **Gross, Dietmar** *(TU Darmstadt)*
Wendland, Wolfgang *(U Stuttgart)*

S24-01: History of applied mathematics and mechanics

Date: June 2, 2023 11:00-13:00
Room: HSZ/105

On the Invention of Iterative Methods for Linear Systems

Gander, Martin J. *(University of Geneva, Switzerland)* 11:00

Iterative methods for linear systems were invented for the same reasons as they are used today, namely to reduce computational cost. Gauss states in a letter to his friend Gerling in 1823: "you will in the future hardly eliminate directly, at least not when you have more than two unknowns". Richardson's paper from 1910 was then very influential, and is a model of a modern numerical analysis paper: modeling, discretization, approximate solution of the discrete problem, and a real application. The work of Stiefel, Hestenes and Lanczos in the early 1950 sparked the success story of Krylov methods, and these methods can also be understood in the context of extrapolation, pioneered by Bresinzki, a student of Gastinel from Grenoble. This brings us to the modern iterative methods for solving partial differential equations, which come in two main classes: domain decomposition methods and multigrid methods. Domain decomposition methods go back to the alternating Schwarz method invented by Herman Amandus Schwarz in 1869 to close a gap in the proof of Riemann's famous Mapping Theorem. Multigrid goes back to the seminal work by Fedorenko in 1961, with main contributions by Brandt and Hackbusch in the Seventies.

[1] The approximate arithmetical solution by finite differences of physical problems involving differential equations, with an application to the stresses in a masonry dam, Lewis Fry Richardson, Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character, 210, 307-357, 1911.
[2] Über einige Methoden der Relaxationsrechnung, Edouard Stiefel, Z. Angew. Math. Phys. 3, 1-33, 1952.
[3] Über einen Grenzübergang durch alternierendes Verfahren, Hermann A. Schwarz, Vierteljahrsschrift der Naturforschenden Gesellschaft in Zürich 15, 272-286, 1870.
[4] A History of Iterative Methods, Martin J. Gander, Philippe Henry and Gerhard Wanner, in preparation, 2021.

A historical overview of various types of entropy in the mathematical theory of dynamical systems

Gunesch, Roland *(University of Education Vorarlberg, Austria)* 11:40

This talk presents a historical overview of various types of entropy in the mathematical theory of dynamical systems, as well as entropy in the natural sciences, including thermodynamics. The mathematical discussions of entropy include the well-known types of topological entropy and measure-theoretic entropy. There is a discussion of historical roots of the concepts of

entropy in theoretical thermodynamics and connections with modern topics, such as information theory.

In the context of information theory, the classical concept of entropy has gained much importance, and so have the mathematical theories of entropy. Foremost among these is the discussion of entropy in the theory of dynamical systems, where concepts of uncertainty and distribution of ensembles have been formalized and turned into a mathematically rigorous theory.

This talk covers a long history of the use of entropy from the 1850s (Rankine, Clausius) to the most modern applications in the mathematical treatment of Big Data in the 2020s.

History of Mathematics at the University of Freiburg

Kroener, Dietmar *(University Freiburg, Germany)* 12:00

Many impulses and ideas have emanated from Freiburg and results have been achieved for mathematics: The axiom of choice, axiomatic set theory, transcendence of π, the Laplace transformation, solution of Hilbert's 7th problem, Görtler vortices, error estimates for finite elements, interval arithmetic, etc. and the foundation of the Mathematical Research Institute in Oberwolfach. In this contribution, I would like to limit myself to the aspects of applied mathematics at the University of Freiburg in the period from 1933 to 1960, in particular to Gustav Doetsch, Wilhelm Süss and Henry Görtler. Gustav Doetsch was a professor since 1931 and he was employed in the Reich Aviation Ministry. From 1945 up to 1951 he was therefore suspended as a professor in Freiburg especially at the instigation of Wilhelm Süss, one of his main rivals in scientific organization in the Third Reich. Doetsch had denounced Ernst Zermelo, among others, for refusing to begin his lectures with the Hitler salute. In 1933 he welcomed the expulsion of Jewish mathematicians such as his teacher Landau and his coauthor Felix Bernstein from their posts. His opponent Wilhelm Süss prevailed over Doetsch and founded the Mathematical Research Institute in Oberwolfach in 1944. Influenced by the Nazi Zeitgeist, also within mathematics, Görtler published a paper in the journal "Deutsche Mathematik" in 1936, in which he wrote, among other things: "Mathematics in particular has the right to exist when it is a powerful expression of the Nordic-German spirit. Mathematical thinking does not have the right to exist if it originates from an alien and opposing attitude of mind...." Görtler became a research assistant in Prandtl's group in Göttingen until 1944, and as a member of the SA and the NSDAP he was thus actively involved in wartime research. In 1944 he was appointed to the University of Freiburg and was one of the founders of the Mathematical Research Institute in Oberwolfach. The activity in Göttingen and the above-mentioned citation led to Görtler's initial suspension in 1945, and only through the support of some colleagues and queries by the Denazification Commission he was accepted into public service as a professor. His research focused on the instability a boundary layers with respect to three-dimensional perturbations, the Taylor-Görtler vortices. Görtler founded the Institute for Applied Mathematics at the University of Freiburg after the war.

S24-02: History of applied mathematics and mechanics

Date: June 2, 2023 16:00-18:00
Room: HSZ/105

On the lever law of Archimedes in the mechanics of bodies

Balke, Herbert *(TU Dresden, Germany)* 16:00

The lever law of Archimedes (287-212 BC) belongs to mechanics and physics. It is used in practice since the antiquity. Experiments (Recknagel, 1960) confirm the lever law. The physical or the chemical structure of the materials do not influence the lever law. The lever law of Archimedes may be considered as the beginning of statics (Simonyi, 2012; Kurrer, 2016). In physics (Lenk, 1989; Flügge, 1960), the mechanics consists of two parts: Newton's (classical) mechanics of mass-points (Synge, 1960) and continuum mechanics (Truesdell and Toupin, 1960). The first part explains the empirical laws of Kepler by Newton's axioms, law of gravity and the mass-point model of the planets (Newton, 1687; Hund, 1945). The body of finite dimensions remains undefined in Newton's axioms. The balance of moments of forces does not appear in Newton's axioms (Balke, 2005). However, Newton's axioms for systems of mass-points provide a balance of moments of forces. This deduction is not valid for continuous bodies. In continuum mechanics the material body and the mass-point are geometrically independent concepts. The lever is a special material body. Here surface forces and volume forces are allowed besides single forces at rigid bodies. By this and Stevin's vector definition (1608), a three-dimensional generalization of the lever law provides the balance of moments of forces (Euler, 1775). Some books of theoretical physics do not contain continuum mechanics, e. g. Landau, 1987 or Rebhan, 2001. Other books postulate the symmetry of the stress tensor without experimental arguments, e. g. Schmutzer, 2005. Scheck (2007) cites Euler's balance of moment of momentum without information about the title. Older textbooks on theoretical physics explain the global balance of moments of forces on the base of point-mechanics, however without logic arguments, e. g. Joos, 1959, as Truesdell 1964 has shown. Laue already 1921 referred to the problematical reduction of the continuum mechanics to the mechanics of mass-points. Actually, in a standard textbook of physics, Meschede (2015) claims a logical deduction of the continuum mechanics from the point-mechanics. The same book contains elementary shortcomings of the application of the lever law to the shear strength. Similar shortcomings are also found in the science of materials, e. g. Gottstein, 2014. In engineering mechanics, the mixture of point- and continuum mechanics provides contradictions in the base assumptions (Hibbeler, 2012; Hauger et al., 2002). The original version of the lever law remains untouched.

A short Historical Review on Porous-media Research

Ehlers, Wolfgang *(University of Stuttgart, Germany)* 16:40

In porous-media research, multi-physical problems occur, whenever different materials (solids, liquids, gases) frequently interact. In soil mechanics as well as in the mechanics of biological

tissues and various other applications, where porous solids are filled with fluids, this interaction takes place on the micro-structure of the material and has to be homogenised towards macroscopic approaches. As a result, the computation of multi-physical and multi-component problems is based on the assumption of superimposed and interacting continua embedded in the well-founded Theory of Porous Media (TPM). The lecture aims at presenting a historical overview of porous-media research ranging from the early days of Darcy and Fick via the Austrian protagonists Terzaghi and Fillunger and classical work by Biot and Truesdell towards modern continuum mechanics of multicomponent materials by Bowen, de Boer and many others. Once porous-media theories are established resulting in a set of strongly coupled partial differential equations (PDE), the computation of realistic problems can be achieved by numerical schemes like the finite-element method (FEM) combined with monolithic solution techniques.

From beam to plate bending

Kienzler, Reinhold *(University of Bremen, Germany)* 17:00

Interest in a theory for vibrating plates arose form Chladni's "Klangfiguren". We follow the engineering and variational attempts of Bernoulli, Germain, Kirchhoff, Reissner and others, and end with the consistent approximation aopproach used in recent years.

The study program “Dynamics and Strength of Machines” in the formerly USSR

Altenbach, Holm *(Otto-von-Guericke-Universität Magdeburg, Germany)* 17:20

In the second half of the 20th century, in the former Soviet Union, an attempt was made to establish a study program in the field of mechanics that also took into account the interests of industry in particular. This meant that an independent study program had to be developed, which differed significantly from the “Mechanics” study programs in traditional universities. The specifics of the new study program are presented using selected examples. At the same time, the corresponding study programs in the Federal Republic of Germany and the former GDR are briefly compared and discussed.

S25: Computational and mathematical methods in data science

Organizer(s): **Pietschmann, Jan-Frederik** *(TU Chemnitz)*
Stoll, Martin *(TU Chemnitz)*

S25-01: Computational and mathematical methods in data science

Date: May 31, 2023 08:30-09:30
Room: POT/112

Linearized unbalanced optimal transport

Schmitzer, Bernhard *(Uni Göttingen, Germany)* 08:30

Optimal transport provides a geometrically intuitive Lagrangian way of comparing distributions by mass rearrangement. The metric can be approximated by representing each sample as deformation of a reference distribution. Formally this corresponds to a local linearization of the underlying Riemannian structure. When combined with subsequent data analysis and machine learning methods this new embedding usually outperforms the standard Eulerian representation. In this talk we recall the linearized optimal transport framework, give some example applications, show how it can be extended to unbalanced transport, and mention some open research questions.

A Pareto optimal extension of the model-free data-driven approach

Ciftci, Kerem *(Ruhr-Universität Bochum, Germany)*
Hackl, Klaus *(Ruhr-Universität Bochum, Germany)* 09:10

The model-free data-driven computational mechanics, first proposed by Kirchdoerfer and Ortiz, has recently emerged in various applications. The approach allows numerical simulations based on data sets of representative samples in stress-strain space without proposing a specific constitutive model. The data-driven paradigm generally solves a multi-objective optimization problem to find material states that satisfy the compatibility and equilibrium conditions while being closest to the given data set. Due to the paradigm relying on nearest-neighbor data clustering, the accuracy of the data-driven simulations depends heavily on the data quality. This study presents a Pareto formulation of the model-free data-driven approach. We define weighted objective functions corresponding to the physical governing equations on the one hand and the distance to the data sets on the other hand. It allows us to search for additional states that satisfy the governing equations in a weak sense but are closer to the given data set. We calculate the solution for the linear combination of the two objectives using physics-informed neural networks. The optimum solution is called the Pareto optimum. In particular, having a fixed number of data points, there is not a single Pareto optimum but a set of different trade-offs between the objectives. Utilizing different weights results in a set of optima forming the so-called Pareto frontier. We give numerical examples to demonstrate the operability of the approach.

S25-02: Computational and mathematical methods in data science

Date: May 31, 2023 14:00-16:00
Room: POT/13

Computability of Optimizers

Lee, Yunseok *(Mathematical Institute, Ludwig-Maximilians University of Munich)* 14:00
Boche, Holger *(Institute of Theoretical Information Technology, Technical University of Munich; Excellence Cluster Cyber Security in the Age of Large-Scale Adversaries, Ruhr University Bochum; Munich Center for Quantum Science and Technology (MCQST); Munich Quantum Valley (MQV))*
Kutyniok, Gitta *(Mathematical Institute, Ludwig-Maximilians University of Munich; Department of Physics and Technology, University of Tromsø; Munich Center for Machine Learning (MCML))*

In this talk, we will focus on the fundamental limitations imposed by Turing machines to solving optimization problems. For this, we will restrict ourselves to finding an optimizer itself, instead of finding an optimal value of a function since in most applications the optimizer is of significantly more interest. Our results show that for well-known optimization problems, the optimizer is unattainable on Turing machines, and thus also on digital hardware. Furthermore, we prove the more general result that such problems are not Banach-Mazur computable, not even in an approximate sense.

This has far-reaching implications, including the non-existence of a computable stop criterion for iterative methods. Iterative methods, such as gradient descent, are commonly used to solve optimization problems. However, our results show that there is no computable stop criterion or no computable way to choose the corresponding step sizes, which would guarantee an arbitrarily small approximation error.

Our results encompass optimization problems from various fields, including artificial intelligence, financial mathematics, and information theory. Our results have far-reaching consequences regarding the trustworthiness of AI, where the absence of approximation guarantees might imply the absence of rigorous certificates.

Well-Definedness Matters: Solving the Uniqueness Problem in PDE Learning

Scholl, Philipp *(Ludwig Maximilian University of Munich)* 14:20
Bacho, Aras *(Ludwig Maximilian University of Munich)*
Boche, Holger *(Technical University of Munich)*
Kutyniok, Gitta *(Ludwig Maximilian University of Munich)*

Physical law learning is the ambiguous attempt at automating the derivation of governing equations with the use of machine learning techniques. Instead of approximating the solution, the goal of physical law learning is to learn the true law governing a phenomenon, to increase the interpretability and, therefore, trustworthiness of the model. Furthermore, interpretable formulas facilitate an understanding and scientific insights which would be impossible with blackbox models. The current literature focuses solely on the development of methods to achieve this goal, and a theoretical foundation is at present missing. This paper

shall thus serve as a first step to build a comprehensive theoretical framework for learning physical laws, aiming to provide reliability to according algorithms. One key problem consists in the fact that the governing equations might not be uniquely determined by the given data. We will study this problem in the common situation that a physical law is described by an ordinary or partial differential equation. For various different classes of differential equations, we provide both necessary and sufficient conditions for a function to uniquely determine the differential equation which is governing the phenomenon. These results show how common the issue of non-uniqueness is, especially for higher order PDEs. Furthermore, we apply the general results we obtained in the first part to specific families of ODEs, which exhibit a great range of behaviors. Based on our theoretical results we then devise numerical algorithms to determine whether a function solves a differential equation uniquely. Finally, we provide extensive numerical experiments showing that our algorithms in combination with common approaches for learning physical laws indeed allow to determine if a unique governing differential equation is learnt, without assuming any knowledge about the function, thereby ensuring reliability.

Physics-Informed Neural Networks for Material Model Calibration in Structural Health Monitoring

Anton, David *(Technische Universität Braunschweig)* 14:40
Henkes, Alexander *(Technische Universität Braunschweig)*
Wessels, Henning *(Technische Universität Braunschweig)*

The identification of material parameters occurring in material models is essential for structural health monitoring (SHM). Due to chemical and physical processes, building structures and materials age during their service life. This, in turn, leads to a deterioration in both the reliability and quality of the structures. The material parameters indicate possible damage and material degradation, as they directly reflect the resistance of the structure to external impacts. Physics-informed neural networks (PINNs) recently emerged as a suitable method for solving inverse problems, such as the calibration of material models. We further developed PINNs for the calibration of the linear-elastic material model from full-field displacement data and global force data in a realistic regime [1]. The advantage of this method is a straightforward inclusion of observation data. Unlike grid-based methods, such as the finite element method updating approach, no computational grid and no interpolation of the data are required. However, calibrating material models using PINNs is computationally expensive. Moreover, the PINN must be trained completely from scratch for each new full-field displacement measurement, even if the geometry and material of the structure remain unchanged. In our ongoing work, we therefore focus on how to physically inform spiking neural networks (SNNs). This new generation of neural networks has the potential to massively reduce memory and energy consumption when trained on next-generation neuromorphic hardware [2]. The SNN achieves this by introducing temporal and neuronal sparsity. In order to further reduce the computational time, we also investigate parametric PINNs, as proposed in [3]. By using parameterized solutions, the PINN does not need to be completely re-trained for each full-field displacement measurement. The calibration of the material model can thus be drastically accelerated, and information about the material condition can be provided near real-

time. Moreover, we also plan to apply the enhanced PINN to more complex material models, such as those for hyper-elastic and elasto-plastic materials.

References:

[1] D. Anton and H. Wessels, "Physics-Informed Neural Networks for Material Model Calibration from Full- Field Displacement Data," arXiv Preprint, 2022. https://arxiv.org/abs/2212.07723v1 [cs.LG].

[2] A. Henkes, J. K. Eshraghian, and H. Wessels, "Spiking Neural Networks for Nonlinear Regression," arXiv Preprint, 2022. https://arxiv.org/abs/2210.03515v2 [cs.NE].

[3] A. Beltrán-Pulido, I. Bilionis, and D. Aliprantis, "Physics-Informed Neural Networks for Solving Parametric Magnetostatic Problems," arXiv Preprint, 2022. https://arxiv.org/abs/2202.04041v2 [cs.CE].

Adaptive step size control for stochastic optimization

Schiela, Anton *(University of Bayreuth)*
Köhne, Frederik *(University of Bayreuth)*

15:00

The performance of machine learning algorithms crucially depends on the choice of several hyperparameters. Finding good choices often consumes large amounts of human and computation resources. Theoretical guidelines on how to choose good hyperparameters are not practical due to computational expensive or inaccessible quantities. We address this issue by presenting a way to adapt an important hyperparameter, the step size (or learning rate), online, during the run of the optimization algorithm with minimal computational overhead. We give theoretical justification for the proposed method as well as numerical results on large scale machine learning problems. We further derive a connection to the established Barzilai-Borwein step sizes, which also have been applied to stochastic optimization successfully. Finally, we show how similar ideas could be used to adapt other hyperparameters, for example momentum or dampening factors.

Singularities in Principal Geodesic Analysis for Hybrid Mechanical Systems

Schubert, Jenny *(Leibniz University Hannover)*
Steinbach, Marc C. C. *(Leibniz University Hannover)*
Gebhardt, Cristian G. *(University of Bergen)*

15:20

We investigate Principal Geodesic Analysis (PGA) in director based dynamics of mechanical systems with potential applications to motion analysis and model order reduction. PGA generalizes Principal Component Analysis (PCA) to the non-Euclidian setting of Riemannian manifolds where singularities of the required logarithm map may occur, e.g., due to periodicity. The talk addresses our approach to lifting trajectories across singularities for the manifolds $SO(3)$ and S^2, which involves branch switching for the logarithm maps. Our numerical experiments with dynamics of hybrid mechanical systems demonstrate that the approach is well suited for motion analysis but require further development for model order reduction.

A data-driven surrogate model for magneto-static simulations

Niekamp, Rainer *(Universität Duisburg-Essen, Germany)*
Niemann, Johanna *(Universität Duisburg-Essen, Germany)*
Reichel, Maximilian *(Universität Duisburg-Essen, Germany)*
Schröder, Jörg *(Universität Duisburg-Essen, Germany)*

15:40

Although the basic framework of Deep Learning, the neural network, was already outlined in 1940's, Deep Learning is still gaining increasing importance and scientific interest due to new Big Data approaches and growing computing capacities. Deep learning algorithms have been successfully used in numerous applications performing various tasks such as object recognition, approximation, optimization, classification, regression, and prediction.

In recent years, deep neural networks (DNNs) have also emerged in the scientific field of magnetism and magnetic materials. They were applied for modeling complex magnetic material, magnetic field calculations and for the prediction of magnetic field distributions generated by permanent magnets.

In this contribution, a data-driven machine learning method based on Convolutional Neural Networks (CNNs) is proposed for applications in magneto-statics, in particular for the computation of demagnetization- and stray fields. Inside a magnetic solid, magnetic materials generate a demagnetization field or a stray field in the surrounding free space. The calculation of these stray fields can be very time consuming using currently available methods, such as the finite element method (FEM). Therefore, in this work, we propose the use of fast data-driven machine learning algorithms. However, machine learning models require a large amount of training data, which is difficult to compute using current methods such as FEM.

Therefore, in this work, a stochastic model based on Brownian motion is used for data generation. More specifically, an algebraic algorithm based on the evaluation of stochastic transition matrices is applied, which enables the generation of large data sets due to its computational efficiency. Two different neural network architectures are considered for the surrogate models: U-shaped Residual Convolutional Neural Network (UResNet) and a Fourier Convolutional Neural Network (FCNN). Finally, the predictions for in dependent geometries are tested to evaluate the performance of the proposed surrogate models models.

S25-03: Computational and mathematical methods in data science

Date: June 1, 2023 16:00-19:00
Room: POT/13

The Numerical Linear Algebra of Training Gaussian Processes

Stoll, Martin *(TU Chemnitz, Germany)* 16:00

Gaussian processes are crucial in computational statistics and machine learning. In order to tune the hyperparameters the log-likelihood functions needs to optimized. To efficiently compute the optimal parameters we need to solve several challenging problems from numerical linear algebra. We will address current state of the art techniques for solving these problems efficiently.

Spiking Neural Networks for Nonlinear Stochastic Regression

Henkes, Alexander *(TU Braunschweig, iRMB)*
Eshraghian, Jason K. *(University of California, Santa Cruz, Department of Electrical and Computer Engineering)*
Wessels, Henning *(TU Braunschweig, iRMB)* 16:20

Spiking neural networks, also known as the third-generation of neural networks, have the potential to significantly reduce memory and energy usage compared to conventional, second-generation neural networks. This is because they inherit temporal and neuronal sparsity, utilizable by subsequent-generation neuromorphic technology, inspired by the human brain's unquestionable efficiency. We introduce this fascinating technology within continuum mechanics to pave the way for engineering applications [1]. Regression issues, which typically occur in the modeling of engineering sciences, are a barrier to spiking neural networks, as they operate in a binary domain. A framework for regression utilizing spiking neural networks is put forth to solve this issue. Specifically, a network topology that uses spiking neurons' membrane potential is developed for decoding binary spike trains to real numbers. Since this contribution aims to provide a succinct introduction to this novel technology, several distinct spiking neural architectures are constructed, ranging from simple spiking feed-forward to complex spiking long short-term memory neural networks. Furthermore, an extension towards stochastic regression is presented, taking into account the non-differentiability of the spiking network, going beyond gradient-based optimization. Numerous numerical studies are conducted on linear and nonlinear, historydependent material model regression. The suggested framework is significantly more energy efficient while maintaining precision and generalizability, as demonstrated by direct comparison with counterparts of conventional neural networks.

[1] Henkes, A., Eshraghian, J. K., & Wessels, H. (2022). Spiking neural networks for nonlinear regression. arXiv preprint `https://arxiv.org/abs/2210.03515`.

Discovering Asymptotic Expansions of Physical Problems Using Symbolic Regression

Abdusalamov, Rasul *(Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany)* 16:40

Kaplunov, Julius *(School of Computer Science and Mathematics, Keele University, Staffordshire, United Kingdom)*

Itskov, Mikhail *(Department of Continuum Mechanics, RWTH Aachen University, Aachen, Germany)*

Asymptotic modeling plays an important role for a variety of physical problems including the analysis of thin plates and shells, solving the Navier-Stokes equation as well as dispersion of elastic waves in strongly inhomogeneous structures, e.g. see [1-3] and references there in. Quite often it is challenging to identify the effect of small problem parameters as well as to derive their asymptotic expansions of the sought solution. Recently, data-driven methods such as symbolic regression have demonstrated their high efficiency for discovering equations and physical relations [4,5]. This work introduces a new automatic method for the generation of asymptotic expansions. The approach is based on symbolic regression. The aim is to find an asymptotic series in the form that fits the given analytical solution as accurately as possible. Therefore, data is generated from analytical solutions for a chosen small or large parameter. Initially, a two-mass collision problem is discussed for three limiting scenarios. Afterwards, a divergent asymptotic series arising in the implementation of a viscoelastic Kelvin Voigt model is investigated. Finally, Lamb waves propagating in an elastic layer are studied. A good agreement between the asymptotic expansions obtained by symbolic regression and the underlying analytical solutions is demonstrated.

References

[1] Kukavica, I., Reis, E.: 'Asymptotic expansion for solutions of the Navier-Stokes equations with potential forces', Journal of Differential Equations, 2011, 250, (1), pp. 607-622

[2] Aghalovyan, L.A.: 'Asymptotic theory of anisotropic plates and shells' (World Scientific, 2015)

[3] Kaplunov, J., Prikazchikov, D.A., Prikazchikova, L.A.: 'Dispersion of elastic waves in a strongly inhomogeneous three-layered plate', International Journal of Solids and Structures, 2017, 113-114, pp. 169-179

[4] Makke, N., Chawla, S.: 'Interpretable Scientific Discovery with Symbolic Regression: A Review', arXiv preprint `https://arxiv.org/abs/2211.10873`, 2022

[5] Udrescu, S.-M., Tegmark, M.: 'AI Feynman: A physics-inspired method for symbolic regression', Science Advances, 6, (16), eaay2631

A nonlinear spectral core-periphery detection method for multiplex networks

Bergermann, Kai *(Department of Mathematics, Technische Universität Chemnitz, 09107 Chemnitz, Germany)*
Stoll, Martin *(Department of Mathematics, Technische Universität Chemnitz, 09107 Chemnitz, Germany)*
Tudisco, Francesco *(School of Mathematics, Gran Sasso Science Institute, 67100 L'Aquila, Italy)*

17:00

Core-periphery detection aims at separating the nodes of a complex network into two subsets: a core that is densely connected to the entire network and a periphery that is densely connected to the core but sparsely connected internally. The nonlinear spectral method from [F. Tudisco, D. Higham, SIAM Journal on Mathematics of Data Science, 1(2):269-292, 2019] addresses this task for single-layer networks by provably solving a constrained nonconvex optimization problem via a fixed point iteration. The result of this method is a coreness vector indicating the closeness of each node to the core. We generalize this idea to the case of multiplex networks in which the same set of nodes exhibits different connectivity patterns on different network layers. As nodes may belong to the core in some layers but to the periphery in others, the definition of core-periphery structure in multiplex networks is not straightforward. We formulate the problem in terms of a nonconvex multi-subhomogeneous objective function that is based on aggregating the network layers via optimized layer coreness weights. The layer coreness vector is optimized simultaneously with the node coreness vector via an alternating fixed point iteration, for which we prove global optimality and convergence guarantees. Numerical experiments on synthetic and real-world networks illustrate that our approach is robust against noisy layers and outperforms state-of-the-art methods based on multilayer node degrees while improving the degree-based method with the novel optimized layer coreness weights. As the runtime of our method depends linearly on the number of edges in the network it is scalable to large-scale multiplex networks.

Incorporation of physical knowledge into artificial neural networks by physics-based Rao-Blackwellization for mechanical problems

Geuken, Gian-Luca *(TU Dortmund)*
Kurzeja, Patrick *(TU Dortmund)*
Mosler, Jörn *(TU Dortmund)*

17:20

Artificial neural networks (ANNs) and data-driven approaches recently have become very popular methods for solving computational problems. This is also the case in the field of scientific computing and, to be more specific, for the modeling and simulation of physical processes. ANN models provide fast and efficient solutions, where classical models frequently meet computational limits.

Recent advances show that such ANNs benefit from the incorporation of physical knowledge. We do so by adapting the so-called Rao-Blackwell theorem to this purpose [1]. The theorem was established for statistical models and improves an initial estimator. Therein, the conditional average under a sufficient statistic is taken as a new estimator. It can be proven that the

new estimator has less than or equal mean-squared-error compared to the initial estimator, making Rao-Blackwellization a powerful algorithm.

The presented framework allows to utilize physical information such as isotropy, observer invariance or dimensional analysis, replacing the sufficient statistic in the original algorithm. The new algorithm can be combined with various other approaches, such as physics-informed neural networks (PINNs) [2] and constitutional artificial neural networks (CANNs) [3]. It still preserves the optimality condition of the Rao-Blackwellization algorithm.

Different aspects and advantages of the proposed method are discussed in terms of ANN design, data generation and data processing based on various illustrative examples. A simple example of a flow curve prediction via an ANN will introduce the method first. Different improvement strategies are then compared for ANNs predicting elastic and brittle energy proportions based on a variational formulation. Results for a non-sufficient set are presented additionally. How sufficient information can be obtained for characteristic forces is shown by a dimensional analysis of drilled steel bars. Finally, an ANN material model for elasticity is built by incorporating isotropy and observer invariance.

[1] P. Kurzeja, The criterion of subscale sufficiency and its application to the relationship between static capillary pressure, saturation and interfacial areas. Proc. R. Soc. A 472, 20150869, 2016. https://dx.doi.org/10.1098/rspa.2015.0869

[2] M. Raissi, P. Perdikaris and G. E. Karniadakis, Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. J. Comput. Phys. 378, 2019. https://doi.org/10.1016/j.jcp.2018.10.045

[3] K. Linka, M. Hillgartner, K.P. Abdolazizi, R.C. Aydin, M. Itskov, C.J. Cyron, Constitutive artificial neural networks: A fast and general approach to predictive data-driven constitutive modeling by deep learning, J. Comput. Phys. 429, 110010, 2021. https://doi.org/10.1016/j.jcp.2020.110010

Posterior-Variance-Based Error Quantification for Inverse Problems in Imaging

Habring, Andreas *(University of Graz)* 17:40
Holler, Martin *(University of Graz)*
Narnhofer, Dominik *(University of Technology Graz)*
Pock, Thomas *(University of Technology Graz)*

We propose a method for obtaining pixel-wise error bounds in Bayesian regularization of inverse imaging problems. The error bounds are computed based on estimates of the posterior variance. Further, techniques from conformal prediction are incorporated in order to obtain coverage guarantees, without making any assumption on the underlying data distribution. The method is generally applicable to Bayesian regularization approaches, independent, e.g., of the concrete choice of the prior. Furthermore, the coverage guarantees can also be obtained in case only approximate sampling from the posterior is possible. With this in particular, the proposed framework is able to incorporate any learned prior in a black-box manner. Guaranteed coverage without assumptions on the underlying distributions is only achievable since the magnitude of the error bounds is, in general, unknown in advance. Nevertheless,

experiments with multiple regularization approaches confirm that, in practice, the obtained error bounds are rather small. For realizing the numerical experiments, also a novel primal-dual Langevin algorithm for sampling from non-smooth distributions is introduced.

S25-04: Computational and mathematical methods in data science

Date: June 2, 2023 08:30-10:30
Room: POT/13

Koopman-based Modeling at the Molecular Scale

Nüske, Feliks *(Max-Planck-Institute for Dynamics of Complex Technical Systems, Germany)* 08:30

High-resolution computer simulations of macromolecular systems have become a valuable tool for modelers and practitioners in biophysics and biochemistry. Yet, despite the surge in computational power we have witnessed over the last few decades, molecular simulations still suffer from at least three fundamental problems: vast dimensionality of the state space, large gaps between elementary simulation steps and time scales of interest, and modeling uncertainty due to the use of empirical force fields. In the past, simulation protocols were mainly designed on physical intuition, and data used to be analyzed more or less by visual inspection. With the rise of modern data science, the field has dramatically transformed. Though by far not the only successful approach, methods based on the Koopman operator have played a central role in that transformation. Koopman operators go back to the origins of quantum physics in the 1930s, and were then re-discovered for classical dynamical systems in the mid 2000s. In the molecular context, it has been found over the last few years that the Koopman framework provides principled approaches to problems like metastability analysis, model reduction, and long-time prediction of molecular systems. In this talk, I will first provide an overview of the Koopman framework. I will then focus on the variational approach to Markov processes, and the role it has played for the solution of several central problems in the field. Finally, I will discuss a number of recent results, including the use of kernel and tensor-based formats within the Koopman framework.

Equivariant Neural Networks for Indirect Measurements

Heilenkötter, Nick *(Center for Industrial Mathematics, University of Bremen)*
Beckmann, Matthias *(Center for Industrial Mathematics, University of Bremen)* 09:10

In the recent years, deep learning techniques have shown great success in various tasks related to inverse problems, where a target quantity of interest can only be observed through indirect measurements of a forward operator. Common approaches apply deep neural networks in a post-processing step to the reconstructions obtained by classical reconstruction methods. However, the latter methods can be computationally expensive and introduce artifacts that are not present in the measured data and, in turn, can deteriorate the performance on the given task.

To overcome these limitations, we propose a class of equivariant neural networks that can be directly applied to the measurements to solve the desired task. To this end, we build appropriate network structures by developing layers that are equivariant with respect to data transformations induced by symmetries in the domain of the forward operator. We rigorously

analyze the relation between the measurement operator and the resulting group representations and prove a representer theorem that characterizes the class of linear operators that translate between a given pair of group actions.
Based on this theory, we extend the existing concepts of Lie group equivariant deep learning to inverse problems and introduce new representations that are the results of the involved measurement operations. This allows us to efficiently solve classification, regression or even reconstruction tasks based on indirect measurements also for very sparse data problems, where a classical reconstruction based approach may be hard or even impossible. To illustrate the effectiveness of our approach, we perform numerical experiments on selected inverse problems and compare our results to existing methods.

Fast Explainable Fourier-ANOVA Methods for Machine Learning

Nestler, Franziska *(Chemnitz University of Technology)* 09:30

Trigonometric functions can be evaluated efficiently based on the Fast Fourier Transform and related techniques. The computational cost is O($N \log N$), where N is the number of given nodes. Feature maps based on such functions are therefore well suited for big data analysis, where the number of data points is typically very large. However, the size of a full grid of Fourier coefficients grows exponentially with the number of features d and, hence, classical FFT-based methods are only efficient for small dimensions.

Recently, the usage of truncated ANOVA (analysis of variance) decompostions has been proposed. Using small superposition dimensions helps to circumvent the curse of dimensionality. The corresponding feature maps can be applied in various Machine Learning algorithms, such as Least-Squares regression or support vector machines. The ANOVA-idea makes the obtained model interpretable and helps identifying relevant features and connections between them, since Sobol indices and Shapley values are easily determined.

Towards Reliable AI: From Digital to Analog Hardware

Fono, Adalbert *(LMU Munich, Germany)*
Boche, Holger *(TU Munich, Germany)*
Kutyniok, Gitta *(LMU Munich, Germany)* 09:50

Deep Learning (DL) has proven to be successful in a wide range of areas, however, also severe disadvantages of this learning paradigm were discovered. An example is given by the instability towards small perturbations of the input. Methods to alleviate this instability phenomenon have been proposed, however, a full understanding is still missing. An assessment of the limitations of DL is not feasible without taking the utilized computing device into consideration. Our goal is to evaluate DL from the perspective of computability theory. Since the training and execution is typically performed on digital hardware, the limitations of digital hardware also translate to DL. By identifying boundaries of algorithmic computations on Turing machines, we also identify the boundaries of reliable DL. An acknowledged aspect of digital computations is its non-exactness - only rational values can be representented exactly. However, real-world problems typically depend on continuous quantities. Hence, it is important to understand under which circumstances this approximate behaviour leads to correct

results, i.e., the computed output satisfies a worst-case error bound. Otherwise, the output of a computation on a digital machine may be wrong unbeknown to the user. The mathematical theory of Turing machines and computability are the necessary tools to study the reliability of digital computations. Turing machines represent an idealized model of digital computers and thereby allow to study the capabilities and limitations of digital devices. Our focus lies on classification problems which represent a common application class of DL methods. We establish conceptual barriers on the capabilities of algorithms on digital hardware to solve classification problems. Subsequently, we also assess the implications for reliable DL on digital hardware. Thereby, the possibility to recognize 'problematic' inputs autonomously, i.e., inputs that cause an algorithm to fail, is studied as well. Are these constraints connected to the properties of Turing machines or to characteristics of classification tasks? We analyze algorithmic solvability in an analog computation model that is based on exact real number calculations, i.e., real numbers can be processed and stored. The Blum-Shub-Smale (BSS) machine is an idealization of noise-free and exact analog computations. It turns out that the previously observed limitations do not arise in this computation model. Therefore, more powerful and reliable DL can be potentially established in this model. However, further research is necessary to evaluate the capabilities of real-world analog devices like neuromorphic hardware and their performance in comparison with the BSS model.

Aspects of image data preparation to extend a classification scheme for cleaning mechanisms to realistic soils

Golla, Christian *(Technische Universität Dresden, Germany)* 10:10
Boddin, Ludwig *(Technische Universität Dresden, Germany)*
Köhler, Hannes *(Technische Universität Dresden, Germany)*
Rüdiger, Frank *(Technische Universität Dresden, Germany)*
Fröhlich, Jochen *(Technische Universität Dresden, Germany)*

Cleaning is an important process step in the food industry, especially to avoid contamination during the increasingly frequent product changes. Machine equipment is cleaned almost daily, resulting in high environmental and economic costs. An approach to reduce these costs is to perform cleaning simulations, but it is necessary to select appropriate models for the soils. The appropriate model depends on the cleaning behaviour of the soil, i.e., the cleaning mechanism that is active in a given situation.

Recently, the authors developed a neural network-based approach to identify the dominant cleaning mechanism from experimental grey-scale image data. The neural networks were trained and validated with video footage of model soils representing a dominant single cleaning mechanism in a prototypical way. Ongoing research will target the application of the neural networks to more realistic soils where the cleaning mechanism may vary over time depending on the operating conditions. This requires an extension to machine learning methods that can efficiently handle time series data.

The cleaning mechanism can be identified from the image data using two main sources of information. On the one hand, small-scale information such as the evolution of the grey value over time in individual pixels can be used. On the other hand, macroscopic patterns such as wavy surface structure or peeling of larger soil patches provide information about the

cleaning mechanism. The focus of this paper is on data preparation that allows both types of information to be used. Based on the data, a machine learning algorithm is developed for time-resolved determination of the cleaning mechanism. This information is necessary to decide how to perform cleaning simulations of the investigated soils.

S26: Modeling, analysis and simulation of molecular systems

Organizer(s): **Nüske, Feliks** *(U Paderborn)*
Covino, Roberto *(Frankfurt Institute for Advanced Studies)*

S26-01: Modeling, analysis and simulation of molecular systems

Date: May 30, 2023 13:30-16:10
Room: HSZ/403

Designing molecular models with machine learning and experimental data

Clementi, Cecilia *(Freie Universität Berlin, Germany)* 13:30

The last years have seen an immense increase in high-throughput and high-resolution technologies for experimental observation as well as high-performance techniques to simulate molecular systems at a microscopic level, resulting in vast and ever-increasing amounts of high-dimensional data. However, experiments provide only a partial view of macromolecular processes and are limited in their temporal and spatial resolution. On the other hand, atomistic simulations are still not able to sample the conformation space of large complexes, thus leaving significant gaps in our ability to study molecular processes at a biologically relevant scale. We present our efforts to bridge these gaps, by exploiting the available data and using state-of-the-art machine learning methods to design optimal coarse models for complex macromolecular systems. We show that it is possible to define simplified molecular models to reproduce the essential information contained both in microscopic simulation and experimental measurements.

A comparative study of recent deep-learning techniques for identifying collective variables of molecular dynamics

Zhang, Wei *(Zuse Institute Berlin)* 14:10

The dynamics of a complex (e.g. high-dimensional, metastable) molecular system can often be characterized by a few features, i.e. collective variables (CVs), of the system. Thanks to the rapid advance in the area of artificial intelligence, various deep learning-based techniques have been developed in recent years that allow for automatic CV indentification of molecular systems from data. These new techniques open the door to efficient modelling and simulation of complex molecular systems that could not be studied before. In this talk, I will introduce a deep learning-based approach for finding CVs by computing the leading eigenvalues and eigenfunctions of the generator associated to the underlying dynamics. A comparative study of this approach, the approaches utilizing autoencoders, as well as VAMPnets based on transfer/Koopman operator theory, will be presented, with the aim of achieving a better understanding on the recent approaches for CV identification. This talk is based on joint work with Tony Lelièvre, Thomas Pigeon, and Gabriel Stoltz.

Molecular free energy and kinetics from AI-assisted path sampling simulations

Lazzeri, Gianmarco *(Frankfurt Institute for Advanced Studies, Germany)*
Jung, Hendrik *(Frankfurt Institute for Advanced Studies, Germany)*
Bolhuis, Peter G. *(Frankfurt Institute for Advanced Studies, Germany)*
Covino, Roberto *(Frankfurt Institute for Advanced Studies, Germany)*

14:30

Extracting the free energy and kinetic information from equilibrium molecular dynamics (MD) is computationally very expensive. In the typical simulation, most computational resources are invested in sampling thermal fluctuations. However, the interesting dynamics is often determined by rare transitions of a few degrees of freedom. Enhanced sampling methods bias the dynamics by applying non-physical forces to overcome the transition energy barrier. But in this way they compromise the system's kinetics. Transition path sampling (TPS) is an advanced technique for obtaining reactive trajectories as if they were extracted from a long equilibrium simulation. Virtual interface exchange (VIE) allows us to use the short TPS simulations in the reweighted path ensemble (RPE). Here, we show that machine learning can enhance TPS and facilitate the extraction of relevant information about the system. Combined with VIE, we developed a method that returns an accurate RPE with a limited number of trajectories. We illustrate our method on the folding of the mini-protein chignolin: we obtained compatible free energy profiles and transition rates with a fraction of the computational resources of equilibrium MD.

Kernel-Based Approximation of the Koopman Generator for Coarse-Grained Stochastic Dynamical Systems

Nateghi, Vahid *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)*
Nüske, Feliks *(Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg)*

14:50

Much attention recently has been paid toward dimensionality-reduction and model discovery for complex systems. Such systems can not be approximated properly with deterministic dynamics.An extension of Extended Dynamic Mode Decomposition (EDMD) has been introduced in [Klus et al., Physica D (2020)] to approximate the Koopman generator for identification of stochastic dynamical systems. However, selection of basis functions upon which the generator is approximated, can not be formulated and is needed to be set heuristically. By taking advantage of kernel methods introduced in [Klus, Entropy (2020)], we develop a kernel-based data-driven method to approximate the Koompan generator of dynamical systems via Galerkin projection in reproducing kernel Hilbert spaces. The method allows us to identify stochastic differential equations governing the coarse-grained model of a high-dimensional system. Dominant dynamics and metastabilities of the system in the reduced-order space, furthermore, can be obtained by the eigen-decomposition of the coarse-grained generator. We numerically investigate the method using toy models governed by overdamped Langevin dynamics.

Validating Molecular Dynamics (MD) and continuum simulations by calculation of the X-ray and neutron scattering patterns

Majumdar, Arnab *(GEMS at MLZ, Helmholtz Zentrum Hereon)* 15:10
Mueller, Martin *(GEMS at MLZ, Helmholtz Zentrum Hereon; Institute of Materials Physics, Helmholtz-Zentrum hereon GmbH; Institut für Experimentelle und Angewandte Physik (IEAP), Christian-Albrechts-Universität zu Kiel)*
Busch, Sebastian *(GEMS at MLZ, Helmholtz Zentrum Hereon)*

With the advent of new technologies, it has been possible to design new materials through theoretical analysis and simulation. However, these simulations have to be validated by experiments. In this work, we develop a method to validate the structural features in continuum simulations directly on the mesoscopic level with X-ray and neutron scattering experiments. The workflow to compare atomistic computer simulations to scattering patterns is well established: the scattering amplitude of individual atoms is summed, whose positions are obtained from the simulation. This approach fails for larger mesoscopic structures due to the unrealistic computation time required to generate the simulations and scattering pattern on a mesoscopic scale with atomic resolution. We developed a methodology that calculates scattering patterns from a continuum simulation like phase-field modeling, where the material description is continuous instead of a collection of atoms. The approach is validated with simple structures and gradually applied to more complex structures. The long-term goal is to use this technique for the simulation of hydrogen storage materials and validation of the simulations with scattering data.

Rate-limiting recovery processes in neurotransmission under sustained stimulation

Ernst, Ariane *(Zuse Institute Berlin)* 15:30
Unger, Nathalie *(Zuse Institute Berlin)*
Schütte, Christof *(Zuse Institute Berlin; FU Berlin)*
Walter, Alexander *(University of Copenhagen, Department of Neuroscience; Leibniz-Forschungsinstitut für Molekulare Pharmakologie)*
Winkelmann, Stefanie *(Zuse Institute Berlin)*

At chemical synapses, an arriving electric signal induces the fusion of vesicles with the presynaptic membrane, thereby releasing neurotransmitters into the synaptic cleft. After a fusion event, both the release site and the vesicle undergo a recovery process before becoming available for reuse again. Of central interest is the question which of the two restoration steps acts as the limiting factor during neurotransmission under high-frequency sustained stimulation. In order to investigate this question, we introduce a novel non-linear reaction network which involves explicit recovery steps for both the vesicles and the release sites, and includes the induced time-dependent output current. The associated reaction dynamics are formulated by means of ordinary differential equations (ODEs), as well as via the associated stochastic jump process. While the stochastic jump model describes a single release site, the average over many release sites is close to the ODE solution and shares its periodic structure. The reason for this can be traced back to the insight that recovery dynamics of vesicles and release sites are statistically almost independent. A sensitivity analysis on the recovery rates based

on the ODE formulation reveals that neither the vesicle nor the release site recovery step can be identified as the essential rate-limiting step but that the rate- limiting feature changes over the course of stimulation. Under sustained stimulation the dynamics given by the ODEs exhibit transient behavior leading from an initial depression of the postsynaptic response to an asymptotic periodic orbit, while the individual trajectories of the stochastic jump model lack the oscillatory behavior an asymptotic periodicity of the ODE-solution.

S26-02: Modeling, analysis and simulation of molecular systems

Date: May 31, 2023 14:00-16:00
Room: HSZ/403

Optimizing the diffusion of overdamped Langevin dynamics

Lelièvre, Tony *(CERMICS, Ecole des Ponts, Marne-la-Vallée, France; MATHERIALS team-project, Inria Paris, France)*
Pavliotis, Grigorios *(Department of Mathematics, Imperial College, London, United-Kingdom)*
Robin, Geneviève *(CNRS & Laboratoire de Mathématiques et Modélisation d'Évry, Évry, France)*
Santet, Régis *(CERMICS, Ecole des Ponts, Marne-la-Vallée, France; MATHERIALS team-project, Inria Paris, France)*
Stoltz, Gabriel *(CERMICS, Ecole des Ponts, Marne-la-Vallée, France; MATHERIALS team-project, Inria Paris, France)*

14:00

Predicting properties of materials and macroscopic physical systems in the framework of statistical physics, or obtaining the distribution of parameter values for Bayesian inference problems, both rely on sampling high dimensional probability measures. Popular methods rely on stochastic dynamics, in particular Markov Chain Monte Carlo (MCMC) methods. We focus on the overdamped Langevin dynamics, with multiplicative noise (i.e. a position dependent noise), which is ergodic for the target Boltzmann measure. Our objective is to compute, explicitly or numerically, the optimal diffusion function leading to the fastest convergence rate, measured here in terms of the spectral gap of the generator of the dynamics. In particular, we discuss the normalization of the diffusion coefficient, since a too large diffusion coefficient has to be compensated by very small time steps.

More precisely, we formalize the maximization of the convergence rate of the overdamped Langevin dynamics with respect to the diffusion coefficient D as a convex optimization program, and we show its well-posedness. We also propose in low dimensional scenarios a numerical procedure combining a finite element parameterization and an optimization algorithm, to compute the optimal diffusion in practice. The numerical procedure is illustrated on simple one-dimensional examples which show the benefits of having a position-dependent diffusion coefficient. We also study the behaviour of the optimal diffusion in the homogenized limit and show it has an analytical expression, proportional to the inverse of the target density, which is in accordance with various previous heuristics. This simple limiting behaviour can be used as an initial guess in an optimization algorithm, or as a proxy for the optimal diffusion which does not require costly convex optimization procedures.

Efficient estimation of transition rates as functions of pH

Donati, Luca *(Zuse Institute Berlin)*
Weber, Marcus *(Zuse Institute Berlin)*

14:20

The μ-opioid receptors are proteins located on the cell membrane's surface that regulate the body's response to pain in inflamed tissues which are characterized by low pH levels. The activation of opioid receptors is caused by endogenous opioids secreted by neurons; or by

exogenous opioids such as morphine and fentanyl, which are administered to the body either for therapeutic or abusive purposes. Unfortunately, the latter can cause undesirable side effects such as tolerance, addiction, and constipation by activating receptors in healthy tissues characterized by normal pH values. It is therefore important to consider the pH dependence of opioids when developing pharmaceutical drugs in order to minimize the risk of adverse effects. For this purpose, Molecular Dynamics simulations have become an essential tool, as they enable us to understand molecular mechanisms at the atomic level and to estimate the transition rates of association and dissociation processes. However, with regard to simulations whose objective is to determine physical observables as functions of pH, the strategies developed to date, commonly referred to as constant-pH simulations, require considerable computational resources, since at least one simulation must be conducted for each pH value of interest. From a statistical thermodynamic perspective, constant pH simulations sample the Grand Canonical Ensemble, i.e., the collection of Canonical Ensembles weighted according to the pH of the system. By exploiting this property, we have developed a novel approach for estimating the transition rates as functions of pH that requires only the sampling of the most probable Canonical Ensembles, for example, those associated with the protonated or deprotonated states [1]. The simulations are then reweighted in order to construct the Grand Canonical Ensemble distribution for a target pH. During the post-analysis, the Fokker-Planck operator of the system is discretized into a rate matrix by Square Root Approximation [2], and the robust Perron Cluster Cluster Analysis (PCCA+) method [3] is employed to construct a coarse-grained rate matrix containing the association and dissociation rates as functions of pH. We have used the method to investigate the pH-dependence of a ligand-receptor system, however, it can be used to estimate transition rates as functions of other environmental variables, such as the salt concentration and the ion concentration which regulate redox systems.

[1] L. Donati, and M. Weber. In: J. Chem. Phys. 157.22 (2022), p.224103.
[2] L. Donati, M. Weber, and B. G. Keller. In: J. Phys. Condens. Matter 33 (2021), p.11590.
[3] P. Deuflhard and M. Weber. In: Linear Algebra Appl. 398 (2004), pp.161-184.

Stochastic Norton Dynamics for Computing Transport Coefficients

Blassel, Noé *(École des Ponts ParisTech; Inria Paris)* 14:40
Stoltz, Gabriel *(École des Ponts ParisTech; Inria Paris)*

Transport coefficients, which quantify the sensitivity in the response of a thermodynamic system at equilibrium to a non-equilibrium perturbation, constitue an important measure of transport phenomena within a molecular medium, and are related to properties such as self-diffusion, shear viscosity or thermal transport. These can be defined at the macroscopic level as the proportionality constant between the magnitude of a non-equilibrium forcing and the intensity of a resulting flux, in the linear response regime where the size of the perturbation is small.

Molecular dynamics techniques have successfully been applied to the numerical computation of transport coefficients, including a perturbative approach whereby the non-equilibrium perturbation is directly applied at the level of the microscopic dynamics, and the resulting average response flux is measured with respect to the non-equilibrium steady state. However, since small perturbations are generally necessary to induce a linear response, these techniques suffer from large statistical errors, which makes their success reliant on the numerical

integration of long trajectories, at a correspondingly large computational cost. Moreover, these approaches fix the forcing magnitude as the defining non-equilibrium state variable, while there is no apparent reason to do so from the macroscopic description.

The Norton method takes a dual approach whereby the defining non-equilibrium state variable is the response: one can fix the response flux, and measure the average forcing magnitude needed to induce it. In the linear response regime, one expects the proportionality constant to give a reciprocal measure of the transport coefficient. At the level of the microscopic dynamics, this amounts to considering a constrained dynamics evolving on a submanifold of phase space, and where the constraint is applied in the direction of the non-equilibrium forcing. It has been studied by Evans and Morris since 1983 for the computation of transport coefficients, but in a deterministic setting where rigorous mathematical results are lacking.

In this work, we propose a stochastic version of the method, and demonstrate numerically its consistency with the standard approach. We further observe that this consistency extends far outside of the linear response regime, raising the question of full equivalence of non-equilibrium ensembles. The method also displays fast spatial concentration properties in the thermodynamic limit. These in turn have an impact on asymptotic variances for estimators of the transport coefficient, which suggest that the Norton method is, at least in some cases, a more efficient approach to tackle the problem of computing transport coefficients.

Extending the regime of linear response with synthetic forcings

Spacek, Renato *(Inria Paris, France)*
Stoltz, Gabriel *(Inria Paris, France)*
15:00

Transport coefficients, such as the mobility, thermal conductivity and shear viscosity, are quantities of prime interest in statistical physics. At the macroscopic level, transport coefficients relate an external forcing of magnitude η, with $\eta \ll 1$, acting on the system to an average response expressed through some steady-state flux. In practice, steady-state averages involved in the linear response are computed as time averages over a realization of some stochastic differential equation. Variance reduction techniques are of paramount interest in this context, as the linear response is scaled by a factor of $1/\eta$, leading to large statistical error. One way to limit the increase in the variance is to allow for larger values of η by increasing the range of values of the forcing for which the nonlinear part of the response is sufficiently small. In theory, one can add an extra forcing to the physical perturbation of the system, called synthetic forcing, as long as this extra forcing preserves the invariant measure of the reference system. The aim is to find synthetic perturbations allowing to reduce the nonlinear part of the response as much as possible. In this talk, I will present a mathematical framework for quantifying the quality of synthetic forcings, in the context of linear response theory, and discuss various possible choices for them. I will illustrate my analysis with numerical results in low dimensional systems.

Sticky Coupling as a Control Variate for Computing Transport Coefficients

Darshan, Shiva *(Ecole des Ponts, France; Inria Paris, France)*
Eberle, Andreas *(Univerity of Bonn)*
Stoltz, Gabriel *(Ecole des Ponts, France; Inria Paris, France)*
15:20

A standard method to compute transport coefficients is to simulate Langevin dynamics perturbed by a small non-equilibrium forcing up to a time T and time-average over the trajectory a desired observable divided by the magnitude of the forcing, η. Unfortunately, this method suffers from large finite-time sampling bias and variance in the limit of small forcing—on the order of $(T\,\eta)^{-1}$ and $(T\,\eta^2)^{-1}$ respectively. For overdamped Langevin dynamics, we propose a method to reduce the bias and variance of this computation using a version of the reference (unperturbed) dynamics coupled to the perturbed dynamics as a control variate. This coupling is sticky in the sense that the distance between the trajectories of the two dynamic is controlled by a one-dimensional process that is sticky at zero. We will show that when the potential of the dynamics is strongly convex outside a compact, this sticky coupling based estimator's reduces the bias and variance by a factor of η^{-1} compared to the standard method. The case of strongly convex outside a compact potentials includes commonly used systems such as Lennard-Jones particles confined to box by a quadratic potential.

A priori error analysis of periodic Schrödinger equations with analytic potentials

Kemlin, Gaspard *(IANS-NMH, Stuttgart University)*
Cancès, Eric *(CERMICS, ENPC and Inria Paris)*
Levitt, Antoine *(LMO, Université Paris-Saclay)*
15:40

This talk is concerned with the numerical analysis of linear and nonlinear Schrödinger equations with analytic potentials. We introduce a hierarchy (H_A) for A>0 of function spaces of complex-valued 2π-periodic functions on the real line which admit analytic extensions on a horizontal strip of width 2A of the complex plane. We then consider a real-valued function V $\in$ H_B for some B > 0, and the corresponding Schrödinger operator H = $-\Delta$ + V acting on the Hilbert space L^2_per of complex-valued 2π-periodic functions on R. We study the H_A regularity of the solutions to (i) the linear problem Hu = f for a given f $\in$ H_A, (ii) the linear elliptic eigenvalue problem Hu = λu, and (iii) the nonlinear elliptic eigenvalue problem Hu+μu^3 = λu. We also study the rate of convergence of the planewave (Fourier) discretization method for computing numerical approximations of u. While the regularity of V (and f) automatically conveys to u in the linear case (in the sense that e.g. the eigenfunctions of H are in H_A for all 0 < A < B), this is no longer true in general in the nonlinear case. Our results, which can be easily extended to the multidimensional case, are motivated by the numerical analysis of Kohn-Sham density functional theory with entire pseudopotentials such as the ones introduced by Goedecker, Teter, and Hutter, and used in the DFTK software.

S26-03: Modeling, analysis and simulation of molecular systems

Date: June 1, 2023 16:00-19:00
Room: HSZ/403

Accelerating mathematical developments in materials modelling by composable software

Herbst, Michael *(Ecole Polytechnique Federale de Lausanne, Switzerland)* 16:00

Today's ubiquitous data-driven workflows allow scientists to expand the limits of length and time scales in materials simulations. In this setting questions related to the robustness and accuracy of simulation protocols as well as the reproducibility of obtained simulation data are more pressing then ever. Due to the overall complexity of underlying physical models (non-linear PDEs, multi-linear algebra) tackling this issues requires expertise from multiple domains. However, close collaboration of mathematicians, application scients as well as researchers from other domains such as computer science requires software, which can support research thrusts all the way from model problems to full-scale applications. With the aim to overcome this obstacle we started the density-functional toolkit (DFTK, `https://dftk.org`) about four years ago. DFTK is a Julia package for Kohn-Sham density-functional theory (DFT), one of the key simulation methods in the field. With only around 7000 lines of code DFTK is highly accessible to support prototyping of algorithms or novel models. Still, building upon Julia's composable software ecosystem it integrates with standard HPC libraries (MPI, CUDA), such that state-of-the-art research simulation in materials science can be performed as well. Unique features include algorithmic differentiation (the ability to compute arbitrary derivatives of output versus input quantities) and a strong focus on having the implementation guided by the matematical structure of the problem. In this talk I will summarise current challenges in materials modelling and illustrate the capabilities of DFTK to assist mathematical research in the field. For this I will follow along a few recent examples where DFTK has enabled cross-disciplinary advances on error estimation for DFT or the developments of more robust algorithms for self-consistent field problems.

Next-order correction to the Dirac exchange energy of the free electron gas and generalized gradient approximations

Friesecke, Gero *(TU Munich, Germany)*
Carvalho Corso, Thiago *(TU Munich, Germany)* 16:40

A milestone in elevating density functional theory (DFT) from a useful first approximation to a widely applicable quantitative method in electronic structure computations was the development of generalized gradient approximations (GGAs) by Becke (1988) and Perdew, Burke, and Ernzerhof (1996). These allow the exchange-correlation energy density at a point r to depend not just on the local density but also the local density gradient. The B88 and PBE functionals improve the accuracy of total DFT energies for small molecules from 1eV to about 0.2 eV, with a similar improvement per unit cell for solids. We derive the next-order correction to the celebrated Dirac exchange energy for the free electron gas in a box with zero boundary

conditions, which is of the order of the surface area of the box and comes from a boundary layer where the density gradient is of order 1. This correction is missed by current GGAs like B88 and PBE, but is captured exactly by GGAs provided these satisfies a certain integral constraint. The new constraint might thus be of interest for the design of future exchange functionals.

The density-density response function in time-dependent density functional theory: mathematical foundations and pole shifting

Carvalho Corso, Thiago *(Technical University of Munich)*
Dupuy, Mi-Song *(Sorbonne Université)*
Friesecke, Gero *(Technical University of Munich)*

17:00

We establish existence and uniqueness of the solution to the Dyson equation for the density-density response function in time-dependent density functional theory (TDDFT) in the random phase approximation (RPA). Moreover, we show that the poles of the RPA density density response function are forward-shifted with respect to those of the non-interacting response function, thereby explaining mathematically the well known empirical fact that the non-interacting poles (given by the spectral gaps of the time-independent KohnSham equations) underestimate the true transition frequencies. Furthermore, we show that the RPA poles are solutions to an eigenvalue problem, justifying the approach commonly used in the physics community to compute these poles.

Robust Solvers for the Schrödinger Eigenvalue Problem with Long-Range Interactions in Anisotropically Expanding Domains

Theisen, Lambert *(University of Stuttgart)*
Stamm, Benjamin *(University of Stuttgart)*

17:20

This talk considers the linear Schrödinger eigenvalue problem for a non-uniform spatial expansion of the domain (e.g., chain- or plane-like). This setup is a model for a many-particle system in which every particle adds an attractive force to the total external potential. Unlike in the purely periodic case without long-range interactions, the factorization method followed by the directional homogenization can not be applied directly. However, interpreting the potential as a perturbed periodic limit allows for an asymptotic analysis and yields insights into the ground state behavior. We can use these findings for numerical applications to solve the collapsing gap problem. In particular, we can apply the quasi-optimal spectral-shift strategy for inner-outer iterative eigenvalue algorithms and combine it with a two-level domain decomposition method. We numerically test the method's robustness and efficiency for Coulomb- and Yukawa-type interactions.

Exact dissociation of the hydrogen dimer in density functional theory with the particle-hole random phase approximation

Dupuy, Mi-Song *(Laboratoire Jacques-Louis Lions, Sorbonne Université)*
Thicke, Kyle *(Department of Mathematics, Texas A&M University)*

17:40

The ground-state energy of a molecule is defined as the lowest eigenvalue of the many-body electronic Schrödinger operator. As such, its computation is limited to systems with a few

electrons. Thankfully, this energy can be obtained by minimising a functional of the electronic density, i.e. a function of a single space variable. This is the Density functional theory (DFT) [1,2] which constitutes a tremendous reduction of dimensionality. Unfortunately the exact functional is unknown. Approximations have been designed in the last decades based on asymptotics for specific systems and numerical fitting. Despite its success for molecules with hundreds or more electrons, the vast majority of these density functional approximations fails to correctly describe the simplest molecular reaction, i.e. the dissociation of the hydrogen dimer where the hydrogen atoms are pulled apart and sent infinitely far away. In the dissociation limit, the ground-state energy of the molecule is twice the energy of a single hydrogen atom, but numerical experiments suggest that it is borne out only for a few density functional approximations [3], among them the particle-hole random phase approximation (RPA). RPA is an approximation of the correlation energy, which is formally derived using an adiabatic connection between the many-body Schrödinger operator and the Kohn-Sham one. Although it is possible to carry a full minimisation of the functional with the RPA correlation energy, it is used as a correction of another converged calculation, typically a restricted Hartree-Fock calculation.

The aim of the talk is to present a proof of the exact dissociation of the hydrogen dimer [4]. In particular, we show how RPA cancels the spurious self-interaction contribution appearing at the dissociation limit in the restricted Hartree-Fock model. This is a joint work with K. Thicke.

References

[1] Hohenberg, Pierre, and Walter Kohn. Ïnhomogeneous electron gas."*Physical review* 136.3B (1964): B864.

[2] Lieb, E.H. (1983), Density functionals for coulomb systems. Int. J. Quantum Chem., 24: 243-277.

[3] Cohen, A. J., Mori-Sánchez, P., & Yang, W. (2012). Challenges for density functional theory. Chemical reviews, 112(1), 289-320.

[4] Dupuy, M. S., Thicke K. (2022). Dissociation limit of the H2 molecule in the particle-hole random phase approximation. Arxiv preprint `https://arxiv.org/abs/2210.04593`.

Boson peak in disordered materials under shear deformation

Focks, Tobias *(RWTH Aachen University, Institute of General Mechanics)*
Bamer, Franz *(RWTH Aachen University, Institute of General Mechanics)*
Markert, Bernd *(RWTH Aachen University, Institute of General Mechanics)*

18:00

We perform shear deformation protocols on two-dimensional network materials and study the distribution of their vibrational density of states. During the shear deformation process, the vibrational modes of the structure change due to the local change in the shape of the potential energy landscape [1]. We show that one can measure this effect on the difference in the characteristic boson peak, which correlates with numerous features of disordered materials [3]. In this context, quasilocalized and hybridized modes are of particular interest [4,5]. Furthermore, the spectra of eigenvalues can be studied in detail using approaches analog to those in [6]. The overall goal of this study is to gain clarity about the eigenvectors and their change due to load and plastic rearrangements.

Literature:

[1] V. L. Gurevich, D. A. Parshin, and H. R. Schober, Phys. Rev. B, (2005), 014209.
[2] F. Bamer, F. Ebrahem, B. Markert, B. Stamm, Arch. Comput. Methods Eng., (2023), https://doi.org/10.1007/s11831-022-09861-1.
[3] Y.C. Hu, and H. Tanaka, Nat. Phys., (2022), 669-677.
[4] Y. M. Beltukov, C. Fusco, D. A. Parshin, and A. Tanguy, Phys. Rev. E, (2016), 023006.
[5] E. Lerner, and E. Bouchbinder, https://arxiv.org/abs/2210.10326, (2022).
[6] T. Focks, F. Bamer, B. Markert, Z. Wu, and B. Stamm, Phys. Rev. B, (2022), 014105.

Detecting local spots in network materials prone to mechanical failure

Wu, Zhao *(RWTH Aachen, IAM)* 18:20
Bamer, Franz *(RWTH Aachen, IAM)*
Markert, Bernd *(RWTH Aachen, IAM)*

The prediction of the onset of fracture is an ongoing issue in the mechanics of disordered materials. In particular, the fracture process in network glasses, such as silica glass, for example, turns out to be a complex phenomenon that originates from specific spots that have the size of a few hundred atoms only [1]. We show that the local yield stress methods, initially developed for densely packed disordered systems [2], can intriguingly be adapted to predict local spots that will experience material damage caused by external mechanical deformation.

Literature:

[1] F. Bamer, F. Ebrahem, B. Markert, B. Stamm, Arch. Comput. Methods Eng., (2023), https://doi.org/10.1007/s11831-022-09861-1.
[2] S. Patinet, D. Vandembroucq, M.L. Falk, Phys. Rev. Lett. 117 (2016), 045501.

Numerical investigation of the Poisson's ratio of amorphous graphene sheets

Stratmann, Jan *(Institute of General Mechanics - RWTH Aachen University)* 18:40
Bamer, Franz *(Institute of General Mechanics - RWTH Aachen University)*
Markert, Bernd *(Institute of General Mechanics - RWTH Aachen University)*

In 2004, Novoselov et al. [1] experimentally produced graphene consisting of only a few atomic layers introducing 2D materials. Such materials reveal intriguing mechanical phenomena such as extreme tensile strength [2] or negative Poisson's ratios for different 2D crystallographic structures [3]. They also help us understand the mechanical behavior of amorphous networks in general.
We will show that amorphous graphene can reveal auxetic behavior, which can be linked to an out-of-plane flattening effect. Thus, Poisson's ratio is rigorously investigated by numerically producing sets of amorphous graphene sheets with distinct levels of network heterogeneity using an adapted Monte Carlo bond switch algorithm [4]. Using molecular simulations, we submit these sheets to uniaxial tensile loading following the athermal quasistatic (AQS) deformation protocol [5, 6].
We find that the network heterogeneity and the number of layers significantly influence the Poisson's ratio of amorphous graphene.

[1] K. S. Novoselov et al., Science 306 (2004) 666 - 669.
[2] C. Lee et al., Science 321 (2008), 385 - 388.
[3] Z. Gao et al., Nano Lett. 17 (2017), 772 - 777.

[4] D.O. Morley & M. Wilson, J. Phys.: Condens. Matter 30 (2018) 50LT02, 7pp.
[5] F. Bamer et al., Comp. Mater. Sci. 163 (2019), 301 - 307.
[6] F. Bamer, F. Ebrahem, B. Markert, B. Stamm, Arch. Comput. Methods Eng., (2023), https://doi.org/10.1007/s11831-022-09861-1.

S26-04: Modeling, analysis and simulation of molecular systems

Date: June 2, 2023 11:00-13:00
Room: HSZ/403

Fracture Simulations of Polymers: Coupling Molecular and Continuum Models

Weber, Felix *(Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU); Competence Unit for Scientific Computing (CSC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU))*
Bauer, Christof *(Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU); Competence Unit for Scientific Computing (CSC), Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU))*
Ries, Maximilian *(Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU))*
Zhao, Wuyang *(Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU))*
Pfaller, Sebastian *(Institute of Applied Mechanics, Friedrich-Alexander-Universität Erlangen-Nürnberg (FAU))*

11:00

In the context of studying the failure behavior of polymers, insights into molecular phenomena are essential. However, as soon as crack propagation in a classical fracture mechanical setting containing a preinduced crack at the sample surface is to be studied by means of molecular dynamics (MD) simulations, the application of periodic boundary conditions (PBC) is not reasonable. On the contrary, only non-periodic boundary conditions are able to capture this kind of pseudo-experimental setup. Moreover, the considerable computational cost of MD simulations must be addressed to enable the investigation of larger samples. This can be realized by employing multiscale techniques coupling MD and continuum models. An example of such an approach specifically developed in view of amorphous polymers is the Capriccio method. This partitioned-domain approach concurrently couples MD domains with a continuum discretized by the finite element method (FEM). The particle regions and the continuum overlap in a bridging domain, where an energy weighting scheme is utilized. The MD domain is exposed to non-periodic, so-called stochastic boundary conditions (SBC). As part of these boundary conditions, auxiliary particles, the so-called anchor points, are introduced, which transmit the displacements and forces between the finite element (FE) and MD regions. One of our long-term goals is to develop a simulation environment for domain-adaptive crack propagation simulations of polymers using the Capriccio method. Recently, we have developed the movement of the MD domain within the continuum according to the current crack tip position: On the one hand, prior to switching from an FE to an MD description, the corresponding MD system is predeformed to the current deformation state using a hybrid molecular dynamics-continuum mechanical approach, which accelerates the corresponding MD simulation. On the other hand, when switching back to FE, a displacement field obtained from MD using the Murdoch-Hardy approach is applied to the continuum. Moreover, the MD description must cover molecular fracture mechanisms in an appropriate way.

At present, we use a polystyrene model at coarse-grained resolution as a sample system. The corresponding potentials have been obtained by iterative Boltzmann inversion. In current investigations, we are replacing the harmonic bond potentials inherent in the considered system by formulations which are more reasonable for covering bond breakage, such as Morse potentials. With these ingredients at hand, we aim for the simulation of crack propagation pathways accompanied by the calculation of essential properties which can be benchmarked against experimental findings, for instance the energy release rate.

Molecular modeling of disordered solids

Bamer, Franz *(RWTH Aachen University, Germany)* 11:20

Disordered solids are ubiquitous in engineering and everyday use. Since the nature of disorder complicates the realization of physically meaningful continuum-mechanical models, particle-based molecular descriptions provide a powerful alternative [1]. This contribution presents algorithms necessary to numerically generate disordered materials, considering their thermodynamic properties and structural identification. The crucial difference between the shear response of a crystalline and a disordered structure is discussed. In this context, it is elaborated on why it is beneficial to use an overdamped, athermal description to disentangle the complex deformation mechanics of disordered solids, and the theory of the mechanics of disordered materials is discussed, including the problems of prediction and reversibility.

[1] F. Bamer, F. Ebrahem, B. Markert, B. Stamm, Arch. Comput. Methods Eng., (2023), https://doi.org/10.1007/s11831-022-09861-1.

Molecular dynamic study of fracture in silica glass

Shekh Alshabab, Somar *(RWTH Aachen, Chair and Institute of General Mechanics)*
Bamer, Franz *(RWTH Aachen, Chair and Institute of General Mechanics)*
Markert, Bernd *(RWTH Aachen, Chair and Institute of General Mechanics)* 11:40

Disordered solids exhibit intermittent avalanches when slowly driven by an external load. These avalanches are associated in silica glass with plastic rearrangements of the atoms at the nanoscale that manifest as stress and energy drops in the loading curve. The complexity arising from their interactions through long-range elastic fields and the quenched disorder makes statistical approaches suitable for studying their behavior by considering yielding and fracture as a phase transition from the intact to the broken phase. To investigate the avalanche statistics, we perform nanoscale simulations using the athermal quasistatic deformation protocol on inducing fracture to silica glass samples, which were simulated using the melting-quenching technique. We identify and measure the avalanches and damage spots and investigate their evolution in the process of fracture. Our results confirm that the avalanches exhibit scale-free power law statistics, indicative of a critical phenomenon.

Influence of Binding Energies on needed Conditions for Ceramic Formation in Aerosol Deposition

Daneshian, Bahman *(Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Germany)*
Gärtner, Frank *(Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Germany)*
Weber, Wolfgang *(Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Germany)*
Assadi, Hamid *(Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Germany)*
Klassen, Thomas *(Helmut-Schmidt-Universität / Universität der Bundeswehr Hamburg, Germany)*

12:00

In recent years, Aerosol Deposition attracted increasing attention for build-up of ceramic layers. By avoiding phase transformations under solidification from the melt, this solid-state technique can guarantee high phase purity and unique deposit properties. The success in building-up dense layers depends on aerosol particle velocities and sizes, which have to be tuned individually with respect to the ceramic material types. The mechanisms and different influences of material types on layer build-up are still controversially discussed. More recent molecular dynamic simulation models suggested certain types of plastic deformation features as key issue for ceramic particle bonding. However, so far, there is a lack of understanding to which extent the mechanical properties, as a consequence of their intrinsic binding energies, influence the needed impact velocities. In order to address general features, the present study presents results from molecular dynamic single particle impact simulations by varying binding energies and particle sizes. The results show that increasing binding energies from 0.22 to 0.96 eV results in about a factor of three higher velocities (from about 200 to 600m/s) being needed for bonding. Increased particle sizes, here a range from 10 - 300 nm is covered, result in fracture getting more prominent. Despite the simplified 2D approach, this study allows deriving some general trends for successful application of the aerosol deposition method, here coving a material range from silica glass to hard phase tungsten carbide.

Grassmann Extrapolation of Density Matrices for Born–Oppenheimer Molecular Dynamics

Polack, Etienne *(École Nationale des Ponts et Chaussées (ENPC))*
Dusson, Genevieve *(Université de Franche-Comté and CNRS)*
Lipparini, Filipppo *(University of Pisa)*
Stamm, Benjamin *(University of Stuttgart, Germany)*

12:20

Born-Oppenheimer molecular dynamics (BOMD) is a powerful but expensive technique. The main bottleneck in a density functional theory BOMD calculation is the solution to the Kohn-Sham (KS) equations that requires an iterative procedure that starts from a guess for the density matrix. Converged densities from previous points in the trajectory can be used to extrapolate a new guess; however, the nonlinear constraint that an idempotent density needs to satisfy makes the direct use of standard linear extrapolation techniques not possible. In

this contribution, we introduce a locally bijective map between the manifold where the density is defined and its tangent space so that linear extrapolation can be performed in a vector space while, at the same time, retaining the correct physical properties of the extrapolated density using molecular descriptors. We apply the method to real-life, multiscale, polarizable QM/MM BOMD simulations, showing that sizeable performance gains can be achieved. If time permitting, we will also report on the newest developments of providing time-reversible density matrices.

Compressing multireference character of wave functions via fermionic mode optimization

Máté, Mihály *(Chair of Global Analysis, Technical University of Munich, Germany; Theoretical Solid State Physics Department, Wigner Research Centre for Physics, Budapest, Hungary)*
Petrov, Klára *(Theoretical Solid State Physics Department, Wigner Research Centre for Physics, Budapest, Hungary)*
Szalay, Szilárd *(Theoretical Solid State Physics Department, Wigner Research Centre for Physics, Budapest, Hungary; Department of Theoretical Physics, University of the Basque Country UPV/EHU, Bilbao, Spain)*
Legeza, Örs *(Theoretical Solid State Physics Department, Wigner Research Centre for Physics, Budapest, Hungary; Institute for Advanced Study, Technical University of Munich, Germany)*

12:40

The aim of the localization of orbitals in quantum chemistry is twofold. On the one hand, localization leads to chemically intuitive orbitals for rationalizing electronic structure of molecular systems. On the other hand, localized molecular orbitals has proven to be useful in making the high-level correlated quantum chemical methods more tractable computationally. These methods usually involve the optimization of the expectation value of specific physical quantities (e.g., radial extent or charge of the orbitals).
A brief overview of the orbital optimization is presented within the framework of tensor network state (TNS) methods, and demonstrate that it has the potential to compress the multireference character of the wave functions after finding optimal molecular orbitals (modes), based on entanglement minimization. This is the quantum chemical application of the more general fermionic mode transformation [1], which is a joint optimization approach that optimizes both the tensors and the modes simultaneously. This strategy is expected to lead to a routine application of TNS methods for strongly correlated multireference problems.
Numerical simulations have been performed for the nitrogen dimer in the cc-pVDZ orbital set for the equilibrium and for stretched geometries [2].

[1] C. Krumnow, L. Veis, Ö. Legeza, and J. Eisert. Fermionic orbital optimization in tensor network states. Phys. Rev. Lett. 117, 210402 (2016)
[2] M. Máté, K. Petrov, Sz. Szalay, and Ö. Legeza. Compressing multireference character of wave functions via fermionic mode optimization. J. Math. Chem. 61, 362-375 (2023)

S26-05: Modeling, analysis and simulation of molecular systems

Date: June 2, 2023 16:00-18:00
Room: HSZ/403

Nonlinear reduced basis using mixture Wasserstein barycenters: application to an eigenvalue problem

Dalery, Maxime *(Laboratoire de Mathématiques de Besançon, UMR CNRS 6623, Université de Franche-Comté)*
Dusson, Geneviève *(CERMICS, École des Ponts & Inria Paris)*
Ehrlacher, Virginie *(Laboratoire de Mathématiques de Besançon, UMR CNRS 6623, Université de Franche-Comté)*
Lozinski, Alexei *(Laboratoire de Mathématiques de Besançon, UMR CNRS 6623, Université de Franche-Comté)*

16:00

We are interested in the computation of the ground state of a given molecular system with M nuclei characterized by their positions in space and their electric charges. The ground state is the solution to a (possibly nonlinear) eigenvalue problem, often computed using a Galerkin method on a well-chosen basis. The resolution of this problem is in general very costly, especially when the problem is solved for many different geometries, as is the case in molecular dynamics and geometry optimization. In this talk, I will for simplicity focus on a one-dimensional toy problem, which is a linear eigenvalue problem with Dirac delta potentials placed at chosen atomic positions, for which analytic solutions are available [4].

In [3], an interpolation method between solutions for different parameters based on optimal transport was proposed in a different context. However, this method is not expected to scale with the dimension due to the high-computational cost of Wasserstein barycenters, even with most recent algorithms. In this work, we propose a new approach based on a decomposition of the solution as a mixture of Slater functions, for which modified Wasserstein barycenters can be computed efficiently [1, 2]. The method is based on a selection of a few representative solutions using a greedy algorithm in the so-called offline phase, followed by a so-called online phase to compute optimal parameters representing the current solution as a barycenter of selected solutions. Our approach will be illustrated with a few numerical results.

References

[1] J. Delon and A. Desolneux, *A wasserstein-type distance in the space of gaussian mixture models*, SIAM Journal on Imaging Sciences, 13 (2020), pp. 936-970.

[2] G. Dusson, V. Ehrlacher, and N. Nouaime, *A wasserstein-type metric for generic mixture models, including location-scatter and group invariant measures*, arXiv preprint `https://arxiv.org/abs/2301.07963`, (2023).

[3] V. Ehrlacher, D. Lombardi, O. Mula, and F.-X. Vialard, *Nonlinear model reduction on metric spaces. application to one-dimensional conservative pdes in wasserstein spaces*, ESAIM : Mathematical Modelling and Numerical Analysis, 54 (2020), pp. 2159-2197.

[4] D. H. Pham, *Galerkin method using optimized wavelet-Gaussian mixed bases for electronic structure calculations in quantum chemistry*, PhD thesis, Université Grenoble Alpes, 2017.

On the Well-Posedness of the Discrete Single-Reference Coupled Cluster Equations

Hassan, Muhammad *(Sorbonne Université, CNRS, Université Paris Cité, Laboratoire Jacques-Louis Lions (LJLL), 75005 Paris, France)*
Maday, Yvon *(Sorbonne Université, CNRS, Université Paris Cité, Laboratoire Jacques-Louis Lions (LJLL), 75005 Paris, France)*
Wang, Yipeng *(Sorbonne Université, CNRS, Université Paris Cité, Laboratoire Jacques-Louis Lions (LJLL), 75005 Paris, France)*

16:20

Coupled cluster methods are widely regarded as among the most effective algorithms for high precision resolution of the ground state energy of the electronic Schrödinger equation in the dynamical correlation regime. Despite their ubiquitous usage as "gold-standard" methods in quantum computational chemistry, the numerical analysis of the coupled cluster methodology is underdeveloped. The existing analysis relies on a local, strong monotonicity property of the coupled cluster function that is valid only in a perturbative regime, i.e., when the sought-after coupled cluster solutions are sufficiently close to zero. This restriction creates considerable difficulty in deriving *quantitative* error estimates for coupled cluster methods in many practical examples. In order to remedy this situation, we have recently proposed a new well-posedness analysis for the continuous (infinite-dimensional) single-reference coupled cluster method based on the invertibility of the coupled cluster Fréchet derivative. A key advantage of our approach is that it is valid even in non-perturbative regimes and can therefore potentially be used to derive quantitative error estimates in situations where local monotonicity cannot be shown to hold. The aim of the current talk is to describe extensions of our approach to certain classes of *discrete* single-reference coupled cluster equations. As we shall show, this extension involves establishing a discrete inf-sup condition for the coupled cluster Fréchet derivative which presents a challenge due to the non-symmetric nature of the underlying linear operator and the fact that the Laplace operator has an essential spectrum on the unbounded Euclidean space.

Density fitting for clusters of rigid molecules in the context of QM/MM simulations

Lygatsika, Ioanna-Maria *(Laboratoire Jacques-Louis Lions, Sorbonne Université)*
Maday, Yvon *(Laboratoire Jacques-Louis Lions, Sorbonne Université)*
Piquemal, Jean-Philip *(Laboratoire de chimie théorique, Sorbonne Université)*
Lagardère, Louis *(Laboratoire de chimie théorique, Sorbonne Université)*

16:40

In this work, we study intermolecular (non-covalent) interactions in large molecular clusters, consisting of identical molecules, called fragments. The frozen-core approximation is assumed, in which atomic orbitals corresponding to core electrons of fragments remain fixed throughout electronic structure calculations. The goal of this work is to efficiently compute frozen-core intermolecular contributions (Coulomb and exchange repulsion) for all fragments in the cluster, where the electronic density of each fragment is assumed to be independent of other fragments positions. The quantities to evaluate are four-center molecular integrals of electronic densities. The total computational cost scales as N^4, where N is the number of

atomic orbital basis functions on each fragment. In the context of force fields for biomolecular simulations, the Gaussian electrostatic model [1] suggests to reduce this cost using density fit. In this talk, we present a generalised density fit method, for approximating frozen-core intermolecular interaction energies for arbitrary translation and rotation invariant kernel functions. We propose to solve the problem using a greedy strategy, that employs pivoted Cholesky decomposition [2] to construct approximations of orthonormal bases of the vector space in which the electronic density of each fragment lives. Additionally, the number of integrals to evaluate is minimised by truncating the double sum of integral contributions, using Cauchy-Schwarz estimators for integral screening. To achieve the optimal selection of terms to be truncated, the selection procedure is formulated as a resource constrained shortest path problem in a graph, whose exact solution can be obtained using dynamic programming techniques [3]. We show that both procedures of fitting and screening need to be performed only once, at the isolated fragment level. At the cluster level, we provide practical error bounds for the approximation of frozen-core intermolecular interactions for arbitrary displacements and rigid rotations of fragments. The numerical performance of our method is demonstrated on small TIP3P water clusters, for geometries optimised using molecular dynamics. Numerical results show that the cost of our method scales as N^2.

[1] J. Chem. Phys. 125, 184101 (2006)
[2] J. Chem. Phys. 151, 241102 (2019)
[3] European Journal of Operational Research Volume 261, Issue 2, 1 September 2017, Pages 530-539

Domain Decomposition Methods for the Poisson-Boltzmann Equations

Jha, Abhinav *(Universität Stuttgart)*
Stamm, Benjamin *(Universität Stuttgart)*
17:00

Many chemical reactions of interest in chemistry and biology take place in a liquid phase, and it is well noted that the solvent's effects play a crucial role in these processes. There are two widely used classes of models used to account for solvent effects in the computation of the properties of a solvated molecule or ion, namely the explicit solvation models, which adopt the molecular representation of both solutes as well as the solvent, and the implicit solvation models which treat the solute in a microscopic way and the solvent in a macroscopic way. Because of this microscopic treatment, implicit models are computationally more efficient and more popular.

This talk will discuss the domain decomposition methods for implicit solvation models and will mainly focus on the non-linear-Poisson-Boltzmann equations. We will look at the derivation of the method, its implementation and provide some numerical studies.

The domain decomposition X library for continuum solvation models

Nottoli, Michele *(Institute of Applied Analysis and Numerical Simulation, Universität Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart)*
Stamm, Benjamin *(Institute of Applied Analysis and Numerical Simulation, Universität Stuttgart, Pfaffenwaldring 57, 70569, Stuttgart)*
17:20

The computational modeling of molecular systems is a complex task: accurate models usually have a steeply scaling computational cost in the number of modeled atoms, which prevents

their application to large systems. At the same time, most of the interesting chemistry and biochemistry happens in condensed phase, where a proper modeling needs to take into account large regions. A possible solution is to describe in greater accuracy the interesting part, and describe the remaining environment using a simpler and cheaper approach. Provided that the environment is sufficiently homogeneous, it is possible to fully describe it by using only a few macroscopic properties, such as its dielectric permittivity and its ionic concentration. This choice gives rise to the so-called polarizable continuum solvation models[1].

These kinds of models require solving a classical electrostatic problem to be able to fully characterize the effect of the environment on the interesting region. In general, the equations involved are quite simple and well known in the mathematical literature, but at the same time, the domain on which they are defined are rather complicated, thus making the problems difficult. An innovative idea to solve this kind of electrostatic problems is to use the Schwartz domain decomposition technique, thus transforming them into a collection of coupled simpler problems.

In our research group, we implemented domain decomposition methods for three different polarizable continuum solvation models, each of them characterized by different choices in the dielectric permittivity and in the ionic concentration of the environment[2,3,4]. The three implementations, together with the common framework and a custom fast multipole method library, are collected in the domain decomposition X library (ddX)[5].

In this talk, first the three methods are briefly presented, and then the common framework and the library are discussed more in detail. Furthermore, a few examples are shown to describe how the library can be coupled to external computational chemistry packages.

[1]: Tomasi, Mennucci and Cammi, Chem. Rev. 2005
[2]: Cancès, Maday and Stamm, J. Chem. Phys. 2013
[3]: Stamm, Cancès, Lipparini and Maday, J. Chem. Phys. 2016
[4]: Quan, Stamm and Maday, SIAM J. Sci. Comput. 2019
[5]: `https://github.com/ddsolvation/ddX/`

List of authors