94th Annual Meeting

of the Association of Applied Mathematics and Mechanics

March 18th–March 22nd, 2024
Magdeburg (Germany)

Book of Abstracts

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MAX PLANCK INSTITUTE
FOR DYNAMICS OF COMPLEX
TECHNICAL SYSTEMS
MAGDEBURG

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Contents

Prandtl Memorial Lecture and Plenary Lectures

PML: Turbulent-laminar patterns

Speaker: **Tuckerman, Laurette** ***(Sorbonne Université)***
Date: March 18, 2024 14:00–15:00
Room: G26/H1
Laudation: Thévenin, Dominique

Experiments and numerical simulations have shown that turbulence in transitional wall-bounded shear flows such as plane Couette and Poiseuille flow frequently takes the form of long oblique bands, if the domains are sufficiently large to accommodate them. At their upper Reynolds-number threshold, laminar regions carve out gaps in otherwise uniform turbulence, thereby forming regular oblique turbulent-laminar patterns with a large spatial wavelength.
At the lower threshold, isolated turbulent bands sparsely populate otherwise laminar domains and complete laminarization takes place via their disappearance characterized by the 2D directed percolation scenario.

PL1: Nonlocal interaction problems with anisotropy

Speaker: **Mora, Maria Giovanna** ***(Università di Pavia)***
Date: March 18, 2024 15:00–16:00
Room: G26/H1
Chair: Conti, Sergio

Nonlocal interaction energies play a pivotal role in describing the behaviour of large systems of particles, in a variety of applications ranging from biology to physics and materials science. A fundamental question is understanding the optimal arrangement of particles at equilibrium, which are described, at least in average, by minimisers of the energy. Traditionally, the focus of the mathematical literature on nonlocal energies has been on radially symmetric potentials, which model interactions depending on the mutual distance between particles. On the other hand, the mathematical study of anisotropic potentials has been very limited until recently, despite their natural occurrence in modelling systems of particles where a preferred direction of interaction is present. In this lecture I will review some classical results for radially symmetric interactions and I will discuss some more recent results shedding light on the role of anisotropy on optimal distributions.

PL2: Contributions of 4D imaging in mechanics of materials

Speaker: **Hild, François** ***(LMPS / ENS Paris-Saclay)***
Date: March 19, 2024 11:00–12:00
Room: G26/H1
Chair: Hartmann, Stefan

3D imaging (e.g., via x-ray tomography) has become popular for analyzing material microstructures and quantifying their temporal changes. When time lapse series of 3D pictures are acquired during a

single experiment, it is possible to measure displacement fields via digital volume correlation (DVC), thereby leading to 4D results. Such 4D analyses have been performed for more than one decade in the field of mechanics of materials.

The presentation aims at reviewing the achievements of and challenges faced by such measurement technique. A general and unified DVC framework is introduced and its extension to 4D spacetime registrations is discussed. The analysis of in-situ experiments illustrates how mechanically relevant parameters are extracted and how models may be validated. The current challenges are examined and some propositions are given to address them.

PL3: Enforcing physics structure in scientific machine learning: The role of projection-based reduced-order modeling

Speaker: **Willcox, Karen E.** ***(University of Texas at Austin)***
Date: March 19, 2024 12:00–13:00
Room: G26/H1
Chair: Faßbender, Heike

Surrogate modeling plays a critical role in achieving design, control and uncertainty quantification for complex systems. It is also a key enabling technology for predictive digital twins. This talk discusses recent work that combines classical ideas from projection-based reduced-order modeling with a data-driven scientific machine learning perspective. The result is a scalable, non-intrusive, physics-informed approach to surrogate modeling. Rather than learn a generic approximation with weak enforcement of the physics, as in other machine learning approaches, we learn low-dimensional operators of a dynamical system whose structure is defined – through the lens of projection – by the physical problem being modeled. The talk will highlight the importance of embedding this physics structure, especially for challenging problems in engineering where training data are sparse and expensive to acquire.

PL4: Dynamics and control of aerial manipulation

Speaker: **Beitelschmidt, Michael** ***(TU Dresden)***
Date: March 21, 2024 11:00–12:00
Room: G26/H1
Chair: Eberhard, Peter

Unmanned automated aerial vehicles (UAV) have developed rapidly in recent years and are already available on the consumer market as camera drones and toy drones. They are also used in professional environments for monitoring and inspection tasks. Future applications include transport and delivery drones, agricultural drones and passenger transport. “Aerial manipulation", in which robotic tasks are carried out from hovering UAV platforms, is currently developing as a new field of application.

The principle of the rigid multicopter has proven itself for most of the tasks mentioned. Here, several rotors (propellers) are attached to a platform and all flight manoeuvres can be performed by varying the speed and thus the thrust of the rotors.

The frequently used quadrocopter is under-actuated and unable to apply forces and torques in all directions from its initial position. This can only be achieved with fully actuated devices that have at least 6 rotors or active tilt rotors. For this reason, such UAVs are particularly suitable as platforms for manipulation tasks.

Aerial manipulation requires new types of UAVs that are specially designed for this task. This applies to the hardware on the one hand, but in particular to the guidance, navigation and control (GNC). While a classic drone mainly has position and speed control, manipulation tasks also require forces to be controlled in certain spatial directions. In addition, a manipulation task can consist of different phases with different kinematic configurations and changing controller structures. An overview of aerial manipulation tasks currently under development is given. The mounting of a screw by a fully-actuated hexacopter is shown as an example of an air manipulation task.

PL5: Conquering the quantum world: old problems and new challenges for the applied mathematics community

Speaker: **Cancès, Eric** ***(Ecole des Ponts ParisTech and INRIA Paris)***
Date: March 21, 2024 12:00–13:00
Room: G26/H1
Chair: Friesecke, Gero

In a seminal article in 1929, P.A.M. Dirac wrote: "The underlying physical laws necessary for the mathematical theory of a large part of physics and the whole of chemistry are thus completely known, and the difficulty is only that the exact application of these laws leads to equations much too complicated to be soluble. It therefore becomes desirable that approximate practical methods of applying quantum mechanics should be developed, which can lead to an explanation of the main features of complex atomic systems without too much computation."

This quote is more relevant than ever now that modern model order reduction and numerical methods (e.g. reduced bases combined with a posteriori error estimators, geometric optimization methods, hierarchical tensors, randomized linear algebra, quantum embedding methods...) combined with current or expected computing power (exascale computers, quantum computers) are opening new perspectives. This field of research is generating intense activity in computational physics, chemistry and materials science, and it is vital for our community not to miss out on this essential field of research for addressing the scientific challenges of the 21st century (energy production and storage, drug design, atomic and molecular-scale engineering...).

In this lecture, I will illustrate the richness of this scientific field in terms of mathematical and numerical methods, as well as applications, and discuss some current challenges.

PL6: Dynamic fracture simulations with peridynamics and phase-field fracture

Speaker: **Weinberg, Kerstin** ***(University Siegen)***
Date: March 21, 2024 16:30–17:30
Room: G26/H1
Chair: Reese, Stefanie

Peridynamics and phase-field fracture are non-local methods to compute fracturing solids efficiently. While cracks in a solid are sharp two-dimensional interfaces, the phase-field approach regularizes the material discontinuities with smooth transitions between broken and unbroken states. This allows convenient calculations for problems with static or dynamic crack propagation. The deformation and the phase field follow energy optimization but rely on the classical continuum theory to describe the solid.
In contrast, the peridynamic modeling of the body is already based on a non-local description of the continuum. This entails problems, especially with the reproducibility of the classical solutions, but offers a very efficient calculation method for dynamic crack propagation.
In this lecture, both methods will be presented and compared with each other, particularly with regard to dynamic crack propagation. We will study the relationships of critical non-local fracture parameters and focus on the accuracy of the two methods in simulating wave propagation, superposition, and cracking at critical states, e.g., for simulating splintering slices and breaking spaghetti.

PL7: Topological Design Problems and Massive Integer Optimization

Speaker: **Leyffer, Sven** ***(Argonne National Laboratory)***
Date: March 22, 2024 11:00–12:00
Room: G26/H1
Chair: Walther, Andrea

Topological design problems arise in many important manufacturing and scientific applications, such as additive manufacturing and the optimization of structures built from trusses. Topology design optimizes the material layout within a design space to satisfy given global load constraints and boundary

conditions, represented by partial differential equations (PDEs). Traditionally, the PDEs have been discretized using the finite-element method with additional continuous variables that model the density of the material within each finite element, giving a (discretized) layout of the material.

In contrast, we model the material layout using binary variables to represent the presence or absence of material in each finite element. This approach results in a massive mixed-integer nonlinear optimization (MINLO) problem, where the nonlinearities arise from the discretization of the governing PDEs. At first sight, such an approach seems impractical, because it requires a massive number of binary variables (one per finite element): the number of binary variables is driven by the accuracy requirements of the finite-element discretization. We show empirically that traditional MINLO algorithms that search a branch-and-bound tree cannot solve these topology optimization problems with even a coarse finite-element discretization.

Recently, a new class of methods have been proposed for solving MINLOs that arise from the discretization of differential equations. These methods solve a single continuous relaxation of the MINLO, which relaxes the integrality requirement on the binary variables. Given the optimal solution of this relaxation, we apply a rounding technique that relies on space-filling curves. These rounding techniques have a remarkable convergence property, and can be shown to asymptotically converge to the global optimum as we refine the finite-element mesh. We illustrate these solution techniques with examples from topology optimization arising in the design of electro-magnetic cloaking devices.

PL8: Mixed-initiative engineering design

Speaker: **Elgeti, Stefanie *(TU Wien)***
Date: March 22, 2024 12:00–13:00
Room: G26/H1
Chair: Kowalski, Julia

Product innovation is a multi-step process: a creativephase where ideas are born, an evaluationphase where the ideas are evaluated, and an implementationphase where these ideas become tangible. While computer-based assistance systems are already available for the latter two phases, creativity is often still considered an exclusively human attribute. However, recent advances in artificial intelligence (AI) have challenged this notion, as creative AI agents are increasingly integrated into our daily lives and have demonstrated their potential to create original content (e.g., ChatGPT, DALL-E, MuseNet, DeepDream). In light of these advances, a new field of research has emerged in the area of AI-enabled design processes, leading to a more-than-human design process in which a computer agent collaborates with a design team to efficiently and creatively explore the entire design space in search of novel design solutions.

To this end, we will demonstrate new technologies, such as how Variational Autoencoders (VAE) can be used to learn low-dimensional, yet feature-rich shape representations. This approach promises significant improvements in both performance and variety of shapes that can be learned. The resulting geometric representation is then incorporated into a shape optimization framework. In addition, we explore the potential of reinforcement learning (RL) as an optimization strategy. RL is based on the trial-and-error interaction of an agent with its environment. As such, RL can be characterized as experience-driven, autonomous learning. While not necessarily superior to classical optimization algorithms (such as gradient-based approaches) for a single optimization problem, based on the existing literature, we expect RL techniques to thrive when recurrent optimization tasks arise.

Minisymposia and Young Researchers Minisymposia

MS1: Distributed Control and Optimization: Theory and Applications

Organizer(s): Flaßkamp, Kathrin *(Saarland University)*
Ebel, Henrik *(University of Stuttgart)*

MS1: Distributed Control and Optimization: Theory and Applications

Date: March 19, 2024 14:00–16:00
Room: G22/105
Chair(s): Ebel, Henrik
Flaßkamp, Kathrin

Distributed optimal feedback control and neural networks

Grüne, Lars; Sperl, Mario 14:00
University of Bayreuth

In this talk we explain why the existence of near-optimal solutions of optimal control problems with an appropriate distributed structure allows for a curse-of-dimensionality-free representation of the solution of the problem with neural networks. Such a representation is needed in particular when the optimal control problem is solved be means of deep reinforcement learning. We present results for the existence of such structures for linear quadratic problems based on suitable graph-theoretic interconnection structures of the dynamics and the cost and illustrate these results by examples.

NMPC for Cyber-Physical Systems – Decentralized Algorithms for Dynamic Real-Time Collaboration

Faulwasser, Timm; Stomberg, Gösta; Engelmann, Alexander 14:20
TU Dortmund University

Core advantages of Model Predictive Control are its applicability to nonlinear multi-input systems with constraints and the variety of tailored numerical algorithms and powerful software tools enabling real-time implementation [1]. Hence the application of MPC to cyber-physical systems (or to multi-agent systems) is of pivotal interest in many application domains such as energy systems, logistics and transport, and robotics [2]. In this talk we present recent results on collaborative distributed NMPC for cyber-physical systems. We discuss a family of algorithms which is based on the decomposition of primal-dual Newton steps arising from Sequential Quadratic Programming (SQP) [3]. We show how the underlying partially separable problem structure translates into partially separable Newton steps which can then be computed in decentralized fashion, i.e., based only on neighbor-to-neighbor communication. We formulate a framework for decentralized real-time iterations in distributed NMPC that allows for local stability guarantees. Our findings are illustrated with several examples including real-time implementations [4].

[1] Gros, S., Zanon, M., Quirynen, R., Bemporad, A., & Diehl, M. (2020). From linear to nonlinear MPC: bridging the gap via the real-time iteration. International Journal of Control, 93(1), 62-80.

[2] Christofides, P. D., Scattolini, R., de la Pena, D. M., & Liu, J. (2013). Distributed model predictive control: A tutorial review and future research directions. Computers & Chemical Engineering, 51, 21-41.

[3] Stomberg, G., Engelmann, A., & Faulwasser, T. (2022). Decentralized non-convex optimization via bi-level SQP and ADMM. In 61st Conference on Decision and Control (CDC), 273-278.

[4] Stomberg, G., Ebel, H., Faulwasser, T., & Eberhard, P. (2023). Cooperative distributed MPC via decentralized real-time optimization: Implementation results for robot formations. Control Engineering Practice, 138, 105579.

Distributed control of nonlinear constrained multi-agent systems: A tracker-planner framework using local model predictive controllers and Voronoi partitions

Köhler, Johannes; Rickenbach, Rahel; Scampicchio, Anna; Zeilinger, Melanie N.; Carron, Andrea 14:40
ETH Zurich

This talk addresses the design of distributed controllers for the coordination of nonlinear constrained multi-agent systems with cooperative goals. An optimization-based control framework is proposed that merges tracking and planning. Furthermore, Voronoi partitions are utilized to achieve efficient collision avoidance and distributed cooperative objectives (coverage or learning unknown environments). Experimental results for coverage control in unknown environments are provided utilizing miniature cars. Key features of the proposed methodology are rigorous closed-loop guarantees and a distributed implementation with limited communication.

Notable challenges in the distributed control of multi-agent systems include: (i) nonlinear constrained dynamics, (ii) collision avoidance, (iii) need for cooperation & coordination to achieve the control goal. Typical control objectives include exploration of the environment, consensus or coverage. Nonlinear dynamics and collision avoidance requirements occur naturally if autonomous robots (aerial, wheeled, or legged) are deployed.

First, we discuss how coordination of nonlinear constrained systems can be achieved using a tracker-planner framework. Specifically, a centralized planner is utilized to compute optimal setpoints for local agents and local controllers are used to track this setpoint. To this end, a model predictive control (MPC) formulation is proposed that achieves setpoint tracking for complex nonlinear dynamics. Key features of this approach are a simple design, local distributed control, applicability to complex nonlinear constrained dynamics, and low communication requirements.

We particularize this approach to solve the coverage control problem, i.e., coordinating multiple agents to optimally cover an area, under initially unknown environments and with collision avoidance constraints. Specifically, we leverage connections to the classical Lloyd algorithm that alternates the computation of a Voronoi partition and a desired setpoint. We achieve collision avoidance by incorporating this Voronoi partition in the MPC formulation. Furthermore, the Voronoi partitions enable a distribution of the coverage control objective. Thus, we achieve the coverage objective by locally optimizing the coverage cost directly in the tracking MPC and communication is only needed to update Voronoi partitions, yielding a “one-layer” approach. We also show that this formulation can be naturally extended to deal with unknown environments by utilizing online learning and an optimistic objective in the local MPC schemes. Finally, we provide hardware results with miniature race cars, demonstrating practicality and efficacy of the overall framework.

A Fixed-Point Iteration Scheme for Sensitivity-Based Distributed Optimal Control

Pierer von Esch, Maximilian; Völz, Andreas; Graichen, Knut 15:00
FAU Erlangen-Nürnberg

The problem of solving large-scale distributed optimal control problems (OCP) frequently arises in the context of iterative distributed model predictive control (DMPC) for multi-agent systems. Besides

approaches such as the alternating direction method of multipliers (ADMM), decentralized dual decomposition, or Jacobi iterations, sensitivity-based approaches represent one possibility to solve such high-scaled OCPs in a distributed and computationally efficient manner. To this end, the local cost functions are extended by linear approximations of the cost functionals of neighboring agents which ensures coordination between agents. The main advantage of this approach is that even for nonlinear OCPs the sensitivities can be calculated in a computationally efficient manner using optimal control theory and that only one neighbor-to-neighbor communication step per iteration is required in which trajectories need to be exchanged between neighbors. In the course of this presentation, a sensitivity-based approach for the distributed solution of multi-agent systems with nonlinear continuous-time dynamics and state/input couplings is derived. Furthermore, a local fixed-point iteration scheme is presented for the efficient solution of the local optimal control problems arising at the agent level. In addition, the convergence of the sensitivity-based algorithm in combination with a finite number of local fixed-point iterations is investigated.The presentation will begin with defining the problem class and the central optimization problem. Subsequently, it is shown how the sensitivities are calculated for the problem at hand and how these sensitivities can be used to realize a distributed optimization algorithm for solving optimal control problems. Furthermore, it is presented how the fixed-point scheme can be used to efficiently solve the local optimization problem. Finally, simulation results for a nonlinear example system are presented. Special attention is paid to the verification of the theoretical convergence properties of the algorithm.

Sensitivity Analysis of the Performance of a Distributed MPC Scheme on an Occupancy Grid in Combination with Priority Rules

Sprodowski, Tobias
Fulda University of Applied Sciences

15:20

The performance of a distributed Model Predictive Control Scheme (DMPC) depends on many parameters, e.g., the prediction horizon length, the design of the cost function with its parameters, the sampling size, a dynamic priority order of optimisation for the agents, internal tolerance parameters of the solver. Suppose the operation space is quantised to attenuate the effort of the communication burden. In that case, more parameters come into play, i.e., the size of the grid cells, and probably reduced communication schemes to ensure the information exchange between the agents. Hence, as these parameters span a multi-dimensional hypercube of parameter values, an efficient sensitivity analysis is beneficial to obtain the optimal parameter setting to prevent a full exploration of the multi-dimensional parameter configuration space. In this scenario, we explore the elementary effects method, also known as the method of Morris, which allows us to explore the optimal parameter setting for a first screening in this spanned parameter hypercube efficiently and systematically. Without prior knowledge, the elementary effect method allows for exploring the impact and coupling of model and input parameters with a reduced number of necessary model runs by changing one factor at a time, i.e., one parameter value. While this method has the drawback of being able to explore only one output parameter, this perfectly matches our scenario due to the restriction to the performance criterion, i.e., the convergence of all distributed agents when they match their target condition. We explore Morris' method in a DMPC setting applied to a set of simulated mobile robots, sharing a quantised operation space and carrying out the optimisation online. We combine this scenario with a set of priority rules to conduct the performance exploration regarding the chosen parameter setting and present the results of the Morris sensitivity analysis demonstrating an efficient sensitivity approach, which could be applied to a variety of DMPC schemes not restricted to robotics only.

Distributed Control Under Attack: Identifying Anomalous Behavior with Inverse Optimal-Control

Ebel, Henrik; Eberhard, Peter
University of Stuttgart

15:40

Distributed control offers plentiful advantages for decision-making in networks of systems as it can work without a central decision-making entity, facilitating flexibility and extensibility. Moreover, it gets rid of the single point of failure that a central decision maker would be. However, in most distributed

control research, a fundamental assumption is that all agents in the network are benevolent, meaning that they are doing their best to fulfill their assigned control task, given the available information from the network. However, if networks of systems are employed in open or uncontrolled environments, where some of the flexibility advantages really come to fruition, malevolent actors may take part in the distributed control task. Thus, this contribution aims to identify anomalous behavior of network agents to be able to single out potential malevolent agents based on observation data. Critically, due to the interconnectedness of networks of systems, it can be particularly hard to identify which system is culpable for reduced overall performance.

The contribution looks at the prototypical task of formation control, which can be interpreted rather generally as a group of systems coordinating their states relative to one another in a cooperative fashion. A possible physical realization is the formation control of mobile robots, which is in the focus of this work since it has practical applications, e.g., for transportation or manipulation tasks. Methodologically, the contribution proposes an inverse optimal-control approach to identify a behavior model for each participating robot using the data communicated on the network. The approach benefits from the fact that, for engineering systems, the physical dynamics of the systems is often known quite well. Therefore, as a behavior model, this work formulates a model predictive control (MPC) problem subject to the known system dynamics but with unknown cost function. Fitting the MPC problem, i.e., the cost function, to the observation data furnishes the behavior model. As this work shows, in some cases of anomalous behavior, the identified cost function can directly be useful to categorize the observed behavior reliably. Moreover, an interesting research question discussed is how well an MPC-based behavior model works when the actual decision-making mechanism employed by the robots is of different structure, e.g., a different distributed MPC scheme or even a controller not in the realm of distributed optimal control. Finally, an outlook is given for identification methods that do not rely on an a-priori model of the system dynamics.

MS2: Hierarchical Modeling in Computational Engineering

Organizer(s): Torrilhon, Manuel *(RWTH Aachen University)*
Giesselmann, Jan *(Technical Universtiy of Darmstadt)*
Kowalski, Julia *(RWTH Aachen University)*

MS2: Hierarchical Modeling in Computational Engineering

Date: March 19, 2024 14:00–16:00
Room: G22/110
Chair(s): Giesselmann, Jan
Kowalski, Julia
Torrilhon, Manuel

Adaptive Hierarchical Modeling of Friction

Rademacher, Andreas 14:00
University of Bremen

We consider Signorini's problem with friction. Our reference friction law is a nonlinear one based on the work of Betten, which behaves for small contact stress like Coulomb's law and for high contact stress like the one of Tresca. The numerical effort for treating Coulomb's and especially Tresca's friction law is much smaller than for the nonlinear one of Betten. Hence, we want to choose the friction law in the computation adaptively.

In this talk, we focus on the model adaptive algorithm and its two main ingredients: The a posteriori error estimator and the strategy for choosing the model. We derive the a posteriori error estimator using the dual weighted residual (DWR) technique considering user-defined nonlinear quantities of interest. The main challenge is to handle the non-smoothness of the underlying frictional contact problem. That is why we introduce a special linearization technique in the derivation. The adaptive strategy has to take into account the localized estimated error and the mechanical contact situation in order to achieve an efficient model distribution. We present our algorithmic approach to handle these two demands.

Finally, we discuss some numerical results concerning the model adaptive algorithm substantiating the efficiency and the accuracy of it. Furthermore, we give a short outlook on the integration of mesh adaptivity into the presented approach and on the application on realistic problems from the field of sheet-bulk-metal-forming.

Dual based and goal oriented adaptivity by means of upwind and downwind approximations

Mahnken, Rolf 14:20
Paderborn University

Homogenization techniques 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 temporal and mesh adaptivity on the macro scale. 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 primal problem and a user-defined quantity of interest. Due to nonlinearities and time-dependency of plasticity, the estimation of error transport and error generation is often 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. Several numerical examples in

this paper illustrate the effectiveness of the proposed adaptive approach based on downwind approximations in comparison to upwind approximations.

Surrogate models for shape uncertainty quantification

Scarabosio, Laura 14:40
Radboud University, The Netherlands

In this talk, I will discuss strategies to build hierarchies of surrogate models for partial differential equations (PDEs) on parametric domains. Focusing on the case of an elliptic PDE, I will discuss how the parametric representation of the shape of the domain affects the performance of some surrogates. I will then move to interface problems, showing that polynomials surrogates are not well-suited for some quantities of interest and neural networks with ReLU activation function provide instead a viable solution.

On data-driven moment closures for radiative transfer

Schlottbom, Matthias 15:00
University of Twente, The Netherlands

The radiative transfer equation describes the propagation of electromagnetic radiation through a medium, which is relevant for several applications, such as optical tomography techniques. The unknown quantity, i.e., the specific intensity, is defined on a six-dimensional phase-space, consisting of position and velocity variables. One line of classical approaches expands the velocity-dependence of the specific intensity into a power series. The corresponding coefficients in this series, called moments, still depend on position. The radiative transfer equation can then be rewritten as an infinite coupled system of partial differential equations for these moments. Determining the first N moments by using the first N equations is not possible, because higher-order moments are contained in these equations. Finding models for these higher-order moments by the first N moments leads to the so-called moment closure problem. Several approaches have been developed in the past. For example, the PN closure, which simply sets all higher-order moments to zero; or entropy closures, which pose additional constraints by minimizing a functional. In this talk we discuss different approaches that aim to construct moment closures by data-driven approaches.

Hierarchical modelling in benchmarking, analysis and code development for coupled geoprocesses

Nagel, Thomas (1,2); Buchwald, Jörg (2,1); Helfer, Thomas (3) 15:20
1: TU Bergakademie Freiberg
2: Helmholtz Centre for Environmental Research – UFZ
3: CEA, France

In geotechnical safety analyses, process and system understanding need to be demonstrated by numerical simulations of coupled physical phenomena such as multiphase flow, heat transport and geomechanics. Adequacy and utility of such analyses rest, among others, on four pillars: balance-based physical process models, a large number of constitutive relations, a range of methods from numerical mathematics, and the implementation of all former aspects in reliable software.

Rather than basing decisions on full-complexity models alone, a hierarchy of models with increasing complexity is conducive to confidence building from an engineering perspective.
Software development, likewise, can benefit from a clear separation of distinct aspects of the overall models. This implies a reduction of redundancy in code, facilitating in turn software maintenance and quality assurance, as well as hierarchical testing. Verification and validation must encompass the entire model chain, starting from experimental data used for calibration, over the models themselves implemented in the corresponding software, the final input-based parameterization, to the output and derivation of decision-relevant metrics.

We discuss the links between software architecture, hierarchical process models with different degrees of coupling and process detail, material knowledge management and verification/validation

workflows for safety-critical applications. We highlight systematic approaches to address this challenge including the open-source software packages OpenGeoSys and MGIS/MFront.

As an example we will focus on the discussion of international modelling initiatives linked to the analysis of full-scale heater experiments in clay rock. A process model chain from thermal, coupled thermal-hydraulic and coupled thermal-hydraulic-mechanical will be used. Mechanical processes will be represented in increasing complexity starting from local proxies to full-field models. Aside from physical complexity, geometrical complexity will be varied. Finally, we discuss the importance of dedicated material knowledge management in simulator-agnostic databases.

On the systematic coupling of multiphysics, multiscale, and multidomain problems

Egger, Herbert 15:40
Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria

The integration of multiphysics, multiscale, and multidomain problems poses a significant challenge in computational engineering. In this talk, we present a mathematical framework for the systematic coupling of such complex phenomena that allows to encode baisc physical principles like energy conservation or entropy production. The resulting systems are amenable to structure-preserving discretization and model order reduction. Moreover, they allow for the consideration of certain quasi-static limits. The general framework will be illustrated by selectic examples.

MS3: Matrix Nearness Problems and Applications

Organizer(s): Voigt, Matthias *(UniDistance Suisse)*
Mitchell, Tim *(Queens College / CUNY)*

MS3: Matrix Nearness Problems and Applications

Date: March 19, 2024 14:00–16:00
Room: G22/111
Chair(s): Voigt, Matthias
Mitchell, Tim

Eigenvalue optimization and matrix nearness problems via constrained gradient systems.

Guglielmi, Nicola (1); Lubich, Christian (2) 14:00
1: Gran Sasso Science Institute, Italy
2: University of Tübingen

We describe an algorithmic approach to a class of eigenvalue optimization problems that uses constrained gradient flows and the remarkable low-rank structure of the optimizers. The eigenvalue optimization problems considered here arise for example in computing complex, real or structured pseudospectra or their extremal points such as those giving the pseudospectral abscissa and radius. These problems (and extensions thereof) appear as the principal building blocks in the two-level approach to various important matrix nearness problems. The problems come in three variants: optimizing eigenvalues over unstructured complex perturbations of a given matrix, over structured perturbations, which are restricted to a given complex- or real-linear subspace of matrices (for example matrices with a given sparsity pattern or matrices with given range and co-range or Hamiltonian matrices) or finally in a mixed form. In all these cases there is a common underlying rank-1 property of optimizers that will be used to advantage in algorithms.

Structured eigenvalue backward errors for rational matrix functions with symmetry structures

Prajapati, Anshul; Sharma, Punit 14:40
Indian Institute of Technology Delhi, India

Let G(z) be an nxn *rational matrix function* (RMF) of the form

$G(z)=\Sigma^{d}_{p=0}\, z^{p}A_{p}+\Sigma^{k}_{j=0}\,(s_j(z)/q_j(z))E_j,$

where A_p's and E_j's are nxn constant matrices, and $s_j(z)$ and $q_j(z)$ are scalar polynomials. G(z) is said to be structured if A_p's, E_j's and rational functions $s_j(z)/q_j(z)$ follow some symmetry structure. Given a structured RMF G(z) and a scalar λ, the problem of computing the nearest (with respect to some norm) structured RMF $\hat{G}(z)$ of which $\lambda$is an exact eigenvalue is called the *structured eigenvalue backward error* of $\lambda$with respect to G(z). Although the eigenvalue/eigenpair backward errors have been well studied for matrix polynomials, there is only a little literature that deals with the perturbation analysis of rational or more general nonlinear eigenvalue problems. Motivated by [1], we derive explicit computable formulas for the structured eigenvalue backward error of RMFs that carry a symmetry structure. These structures include symmetric, skew-symmetric, Hermitian, skew-Hermitian, *-palindromic, T-even, T-odd, *-even, and *-odd structures. We show over various numerical experiments that the backward errors with respect to structure-preserving and arbitrary perturbations are significantly different.

As far as we know, no other work has been done in the literature on the structured eigenvalue backward error of RMF. This work has been communicated for publication [2].

1. S. Bora, M. Karow, C. Mehl, and P. Sharma. Structured eigenvalue backward errors of matrix pencils and polynomials with Hermitian and related structures. *SIAM J. Matrix Anal. Appl.,* 35 (2014), pp. 453–475.

2. A. Prajapati and P. Sharma. Structured eigenvalue backward errors for rational matrix functions with symmetry structures. *arXiv*:2208.13420

Computing sep-lambda, a measure of how close two square matrices are to sharing an eigenvalue

Mitchell, Tim
Queens College, USA

15:00

Given two square matrices, not necessarily the same size, one might ask whether they share an eigenvalue, and if not, how minimally can their coefficients be changed such that the resulting perturbed matrices do have at least one eigenvalue in common. This distance measure, known as sep-lambda, was first considered by Varah in the late seventies and then subsequently studied by Demmel, although they respectively used slightly different definitions. Varah's interest in sep-lambda stemmed from its connection to the sensitivity of solving a Sylvester matrix equation, while Demmel's was due to it arising in the computation of stable eigendecompositions, and subsequently, as a tool to disprove two conjectures in the eighties related to computing the distance to instability of a stable matrix. More recently, it has also been used by others to analyze the stability of invariant subspaces and approximate pseudospectra.

In this talk, we discuss both versions of sep-lambda, and in particular, two radically different approaches to compute Demmel's version of it. The first is due to Gu and Overton and has its roots in a novel but expensive 2D-level-set convergence test originally developed by Gu for estimating the distance to uncontrollability. We then present a new and much faster algorithm using interpolation-based globally certificates, an idea that was first conceived for computing Kreiss constants and provides a much faster convergence test based on approximating certain one-variable functions globally on their finite domain. We discuss how this methodology works as well as its strengths in terms of efficiency and robustness compared to the older 2D-level-set test approach.

Distance to singularity a "common" problem for dissipative Hamiltonian matrix pencils

Mehl, Christian
TU Berlin

15:20

The distance to singularity for dissipative Hamiltonian pencils, i.e. pencils underlying a linear port-Hamiltonian system, is considered. It is shown that this distance can be interpreted as the distance to a common kernel of the matrix coefficients of the considered matrix pencil. An outlook is given how these results can be generalized to the case of infinite-dimensional systems.

Nearest singular pencil via Riemannian optimization

Dopico, Froilan (1); Noferini, Vanni (2); Nyman, Lauri (2)
1: University Charles III of Madrid
2: Aalto University, Finland

15:40

It was recently observed by Noferini and Poloni [Numer. Math. 148(4), 817–851, 2021] that the problem of finding the nearest stable matrix, i.e., the matrix nearest to a given one whose all eigenvalues lie in a certain set Ω, can be efficiently solved using Riemannian optimization. In this talk, I plan to discuss why and how this idea can be extended to find the nearest singular pencil to a given one. This task is relevant for several applications such as algebraic-differential equations or nonlinear eigenvalue problems, and it can be seen as a constrained optimization problem where the objective function is the Euclidean distance and the constraint is that the optimizer must be a singular pencil, that is, its determinant must be the identically zero polynomial.
The underlying idea is relatively simple: thanks to the generalized Schur form of a pencil, the original problem is equivalent to a minimization task over the Cartesian product of the manifold of unitary matrices with itself. While the new problem is unconstrained, the problem remains difficult due the fact that the underlying geometry is no longer Euclidean; nevertheless, the existing technology for Riemannian optimization can be exploited. Numerical experiments suggest that the resulting algorithm outshines its predecessors in terms of asymptotic complexity. This allows us, for the first

time, to tackle this problem for pencils whos size is not extremely small. Furthermore, the algorithm can be adapted to find the nearest singular pencil with specified right minimal index.
The talk is based on joint work with F. Dopico and L. Nyman and on the preprint https://arxiv.org/pdf/2308.12781v1.pdf

MS4: Kernel Methods in Data Analysis and Computational Science

Organizer(s): Uschmajew, André *(University of Augsburg)*
Garcke, Jochen *(Universtität Bonn)*

MS4: Kernel Methods in Data Analysis and Computational Science

Date: March 19, 2024 14:00–16:00
Room: G22/112
Chair(s): Garcke, Jochen
Uschmajew, André

Gaussian Process Surrogate for Bayesian Parameter Estimation Involving Incompressible Fluids

Wendland, Holger (1); Sloan, Ian (2); Le Gia, Quoc Thong (2) 14:00
1: University of Bayreuth
2: University of New South Wales, Australia

Gaussian processes are often used to model physical processes. In this project we seek to model physical process involving the flow of incompressible fluids, using Gaussian processes that respect the incompressibility. The ultimate aim is to employ the Gaussian process as a surrogate for the forward map in Bayesian inverse problems involving incompressible fluids.

How many neurons do we need? A refined analysis for shallow networks trained with gradient descent

Mücke, Nicole; Nguyen, Mike 14:30
TU Braunschweig

We analyze the generalization properties of two-layer neural networks in the neural tangent kernel (NTK) regime, trained with gradient descent (GD). For early stopped GD we derive fast rates of convergence that are known to be minimax optimal in the framework of non-parametric regression in reproducing kernel Hilbert spaces. On our way, we precisely keep track of the number of hidden neurons required for generalization and improve over existing results. We further show that the weights during training remain in a vicinity around initialization, the radius being dependent on structural assumptions such as degree of smoothness of the regression function and eigenvalue decay of the integral operator associated to the NTK.

Some results on the NTK spectrum and spectral bias of neural networks in the kernel regime

Montufar, Guido (1,2) 15:00
1: University of California, Los Angeles, USA
2: Max Planck Institute for Mathematics in the Sciences, Leipzig

I present work characterizing the spectrum of the neural tangent kernel (NTK) of deep feedforward neural networks in the infinite width limit. We express the NTK as a power series with coefficients depending on both the Hermite coefficients of the activation function as well as the depth of the network. Using this, we relate the effective rank of the NTK to the effective rank of the input-data Gram and study the eigenvalues depending on the choice of activation function. Then I discuss some results bounding the difference between the function space trajectory of finite networks trained on finite samples from the kernel dynamics of infinite width and infinite data. An implication of the bounds is that the network is biased to learn the top eigenfunctions of the NTK not just on the training set but over the entire input space. The talk is based on works with Michael Murray, Hui Jin, and Benjamin Bowman.

Kernel Methods for Koopman-based Modeling

Nüske, Feliks
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

15:30

Koopman operator theory [Mezić, 2005] and its main algorithm Extended Dynamic Mode Decomposition (EDMD) [Williams, 2015] has emerged as a powerful modeling approach for complex dynamical systems arising in physics, chemistry, materials science, and engineering. The basic idea is to leverage existing simulation data to learn a linear model that allows to predict expectation values of observable functions at future times. Though the algorithm is conceptually quite simple, its underlying mathematical structure is very rich, and can be used for different purposes including control, coarse graining, or the identification of metastable states in complex molecules and materials [Noé and Clementi, 2017; Klus, FN, Peitz et al, 2020].

The success of the method depends critically on the choice of finite-dimensional Galerkin subspace (called dictionary), which reflects a priori knowledge of the system. Here, kernel methods emerge as very useful, since they allow using a rich dictionary defined implicitly by the data. In this talk, I will begin by giving a brief overview of how kernel methods can be incorporated into the Koopman framework. Subsequently, I will present two recent results: the first is on probabilistic bounds for the estimation error of kernel-based Koopman models from finite data [Phillip, Schaller, Worthmann, Peitz, FN (2023)]. The second is on using low-rank approximations based on Random Fourier Features [FN and Klus (2023)] to apply kernel methods efficiently in the context of molecular simulation.

MS5: Free Boundary Problems in the Sciences: PDE Analysis and Modeling

Organizer(s): Marino, Greta *(University of Augsburg)*
Hensel, Sebastian *(Hausdorff Center for Mathematics, University of Bonn)*

MS5: Free boundary problems in the sciences: PDE analysis and modeling

Date: March 19, 2024 14:00–16:00
Room: G22/120
Chair(s): Marino, Greta
Hensel, Sebastian

A new reformulation of the Muskat problem with surface tension

Matioc, Anca; Matioc, Bogdan 14:00
University of Regensburg

Two-phase flow in porous media are described by the Muskat problem, which is a moving boundary problem purposed originally to describe the interaction of water and oil in an oil sand. In this talk two formulas that connect the derivatives of the double layer potential and of a related singular integral operator evaluated at some density ϑ to the L_2-adjoints of these operators evaluated at the density ϑ' are used to recast the Muskat problem with surface tension and general viscosities as a system of equations with nonlinearities expressed in terms of the L_2-adjoints of these operators. An advantage of this formulation is that the nonlinearities appear now as a derivative. This aspect and abstract quasilinear parabolic theory are then exploited to establish a local well-posedness result in all subcritical Sobolev spaces $W_p^s(\mathbb{R})$ with $p \in (1,\infty)$ and $s \in (1+1/p, 2)$.(Joint work with Bogdan Matioc, Regensburg)

The Mullins–Sekerka equation: Existence theory and weak-strong stability for a novel weak solution concept

Fischer, Julian (1); Hensel, Sebastian (2); Laux, Tim (3); Simon, Theresa (4); Stinson, Kerrek (2) 14:20
1: Institute of Science and Technology Austria
2: University of Bonn
3: University of Regensburg
4: University of Münster

Weak solution theories are in general necessary for interface evolution problems as topology changes naturally occur. If the topology change is realized through a physically unstable singularity, this results in non-uniqueness of solutions afterward. The best one can thus expect is a weak-strong uniqueness principle; and this was proven in recent years for prominent examples (e.g., multiphase mean curvature
flow). At the level of a weak solution concept, the key conceptual ingredient for these results is given by the dissipative nature of the problems.
In the first part of the talk, I will introduce a recently established weak solution theory for a basic example of a higher-order curvature flow: the Mullins–Sekerka equation. This solution theory is essentially only encoded in terms of a single sharp energy dissipation principle, taking direct inspiration from De Giorgi's approach to gradient flows or the Sandier–Serfaty approach to evolutionary Γ-convergence. Furthermore, our solutions satisfy a weak-strong uniqueness principle (and more generally, a weak-strong stability estimate), which is the content of the second part of the talk.
This is joint work with Kerrek Stinson (existence result), and Julian Fischer, Tim Laux and Theresa Simon (uniqueness result).

A Non-local Free Boundary Problem Arising in a Model of Cell Polarization

Logioti, Anna (1); Niethammer, Barbara (2); Röger, Matthias (3); Velázquez, Juan J. L. (2)
1: University of Stuttgart
2: University of Bonn
3: TU Dortmund University

14:40

We consider a model for cell polarization as a response to an external signal which consists of a bulk-surface reaction-diffusion system of equations. We have proved that in a suitable scaling limit the system converges to a non-local free boundary problem. In this talk, I will present several results for this problem, starting with an L1-contraction property and, in the case of time-constant signals, the stability of stationary states. In addition, I will address some qualitative properties of the free boundary. More precisely, we have concluded that there are necessary and sufficient conditions for the initial data that yield continuity of the support at t = 0. If one of these assumptions fail, then jumps of the support take place. We have further provided a complete characterization of the jumps for a large class of initial data.

This is a joint work with B. Niethammer, M. Röger and J. J. L. Velázquez

Phase-Field Models for Organic Solar Cell Production

Tretmans, Carmen; Pietschmann, Jan-Frederik
University of Augsburg

15:00

In this talk, we discuss a model for the formation of acceptor and donor regions during the production of organic solar cells. The process is based on a spinodal decomposition of two species in a solvent, where the solvent is allowed to evaporate. This yields a coupling of the respective phase field equations via a degenerate mobility. We provide some insight on the modelling and the application, as well as several numerical examples based on finite element simulations.

Comparison of the fracture toughness of two species of cactus using phase field modeling

Dondl, Patrick; Mylo, Max; Speck, Olga; Striet, Ludwig
University of Freiburg

15:20

We develop a phase field model to understand the abscission process of different species of cacti. In particular, the cactus species *Opuntia ficus-indica and Cylindropuntia bigelovii* exhibit a vastly different effective fracture toughness, while relying - as all plants do - on a very limited set of basic materials as
building blocks. We thus include the available morphometric and biomechanical data of our cactus species in the variational framework of brittle fracture presented by Bourdin et. al in 2008 and study their behavior compared to fictional cacti to isolate the effect of different geometric, microstructural, and materials features on the effective fracture toughness. The results from finite element simulations of this model are compared to experimental testing. The main motivation of this research is to gain inspiration for novel methods aiding the separation of artificial materials systems to sort raw materials for sustainable reuse and recycling.

A free boundary model for transport induced neurite growth

Marino, Greta (1); Pietschmann, Jan-Frederik (1); Winkler, Max (2)
1: University of Augsburg
2: TU Chemnitz

15:40

We introduce a free boundary model to example the effect of vesicle transport onto neurite growth. It consists of systems of drift-diffusion equations describing the evolution of the density of antero- and retrograde vesicles in each neurite coupled to reservoirs located at the soma and the growth cones of the neurites, respectively. The model allows for a change of neurite length depending on the vesicle concentration in the growth cones. After establishing existence and uniqueness for the time-dependent problem, we briefly comment on possible types of stationary solutions. Finally, we provide numerical studies on biologically relevant scales using a finite volume scheme. We illustrate the capability of the model to reproduce cycles of extension and retraction.

YRM1: Mechanics and Mathematics of Sea Ice

Organizer(s): Mehlmann, Carolin *(Otto-von-Guericke Universität)*
Schwarz, Carina *(University of Duisburg-Essen)*

YRM1: Mechanics and Mathematics of Sea Ice

Date: March 18, 2024 16:30–18:30
Room: G22/020
Chair(s): Mehlmann, Carolin

Recent results in the mathematical analysis of Hibler's sea ice model

Brandt, Felix 16:30
TU Darmstadt

In this talk, we focus on the mathematical analysis of Hibler's sea ice model. First, we describe the approach to interpret the model as a system of quasilinear evolution equations. In a second step, we elaborate on the strategy to obtain local strong well-posedness even without regularization by diffusion in the balance laws. Finally, we also comment on the analysis of a coupled atmosphere-sea ice-ocean model. The talk is based on joint work with Tim Binz and Matthias Hieber.

Advancements in sea ice dynamics modeling based on a mixed least-squares Finite Element study with non-conforming stress approximation

Hellebrand, Sonja; Schwarz, Carina; Schröder, Jörg 16:50
University of Duisburg-Essen

This contribution bases on the established model for sea ice dynamics, which describes the viscous-plastic sea ice behavior at scales spanning several thousand kilometers, cf. [1]. Focus of the numerical model is on the simulation of the sea ice circulation and its evolution over a seasonal cycle. Therefore, it takes into account the sea ice thickness as well as the sea ice concentration. The physical behavior of the later two quantities are governed by transient advection equations, in which the sea ice velocity serves as coupling field.

Recent investigations proposed the finite element implementation of the sea ice model based on a (mixed) Galerkin variational approach, see e.g. [2 and [3]. However, challenges arise in stabilizing the numerically complex scheme, particularly in dealing with the first-order advection equations. In order to address these challenges, the utilization of the mixed least-squares method is promising. One main advantage of this method is its applicability to first-order systems, i.e., it provides stable and robust formulations even for non-self-adjoint operators, such as the tracer equations (for sea ice thickness and sea ice concentration).

The here presented least-squares finite element formulation bases on the instationary sea ice equation, including the balance of momentum and a constitutive law for the viscous-plastic flow. In the utilized mixed least-squares approach four primary fields are considered, which are the stress**,** the velocity, the concentration and the thickness. Four residuals are defined for the derivation of a first-order least-squares formulation based on the balance of momentum, the constitutive relation for the stresses, and two tracer-equations. In comparison to our previous investigations, a distinctive approach is proposed in which the stresses are approximated in a non-conforming manner. Hence, instead of employing H(div) conforming interpolation functions, Lagrange interpolation functions for the stresses are utilized aligning them with the interpolation approach used for other fields. These two approaches are compared analyzing a box test case, see [3], to validate the new approach. Moreover, the results are compared to existing literature.

References:

[1] W.D. Hibler III. A dynamic thermodynamic sea ice model. Journal of Physical Oceanography, 9(4):815–846, 1979.

[2] S. Danilov, Q. Wang, R. Timmermann, M. Iakovlev, D. Sidorenko, M. Kimmritz, T. Jung. Finite-Element Sea Ice Model (FESIM), Version 2. Geoscientific Model Development, 8:1747–1761, 2015.

[3] C. Mehlmann and T. Richter. A modified global Newton solver for viscous-plastic sea ice models. Ocean Modelling, 116:96–107, 2017.

Comparing heterogeneity and Linear Kinematic Features in sea ice models with Viscous-Plastic and Maxwell Elasto-Brittle rheologies

Bourgett, Mirjam (1); Losch, Martin (1); Plante, Matthieu (2)

1: Alfred Wegener Institute Bremerhaven

2: Recherche en prévision numérique environnementale, Environnement et Changement Climatique Canada

17:10

Representing sea ice deformations in large scale climate models is a challenge as the large scale climate models very much depend on smaller-scale physics that are poorly resolved at coarse resolution. Most continuum sea ice models use the viscous-plastic (VP) rheology for quasi-homogenous non-normal fluids. At high resolution, VP models are able to reproduce some of the large scale statistics of sea ice deformations. At coarser resolutions, the scaling properties of sea ice deformations may be inconsistent with observations. Different approaches try to include smaller scale characteristics in large scale sea ice models. New rheologies such as the Maxwell eslasto-brittle (MEB) rheology introduce a parameterisation of damage that represents the presence of sub-grid scale fractures. The new brittle rheologies simulate realistic large scale fields with adequate heterogeneity and intermitency even at coarser grids. Often a given sea ice model code implements only one type of rheology which leads to rheology comparisons that are confounded by numerical discretization, advection scheme, and grid resolution. Here, we add the MEB rheology to the sea ice component of the Massachusetts Institute of Technology general circulation model (MITgcm), which already contains VP-rheologies with many different options and yield curves for the purpose of unconfounded comparisons between sea ice rheologies in a coupled ice ocean framework. Idealised experiments show the credibility of the new code. The spatial heterogeneity, measured by the number of simulated linear kinematic features (LKFs), depends to a large degree on horizontal grid spacing, but also on the parameterisation of sub-grid scale variability for both VP and MEB rheologies. Stochastic parameterisations of mechanical parameters (ice strength, cohesion) are used for the sub-grid scale variability.

Simulating Sea Ice Faster with GPUs

Jendersie, Robert (1); Lessig, Christian (2); Richter, Thomas (1)

1: Otto von Guericke University Magdeburg

2: European Centre for Medium-Range Weather Forecasts

17:30

The cryosphere plays a significant role in the global climate. Therefore, the accurate simulation of sea ice is an important step to improve climate projections. To enable higher resolution climate simulations, graphics processing units (GPUs) have become increasingly attractive, as they offer higher floating point performance and better energy efficiency. However, accessing these theoretical benefits usually requires more care and effort in the implementation. In recent years, an increasing number of frameworks have become available that promise to simplify general purpose GPU programming. In this talk, we look at multiple such frameworks for the parallelization of neXtSIM-DG, a finite-element based sea ice simulation. Besides conventional methods like CUDA and SYCL, we show how the machine learning framework PyTorch may be leveraged to make effective use of GPUs. By re-implementing a representative part of the simulation, we evaluate the different approaches according to their usability and performance.

A model for ice-mélange based on particle and continuums mechanics

Kahl, Saskia; Mehlmann, Carolin

Otto von Guericke University Magdeburg

17:50

Ice mélange (a mixture of sea ice, bergy bits and icebergs) can have a strong influence on the sea-ice–ocean interaction. So far, ice mélange is not represented in climate models as numerically efficient

realizations are missing. This motivates the development of an ice-mélange model based on the viscous-plastic sea-ice rheology, which is currently the most commonly used material law for sea ice in climate models. Starting from the continuum mechanical formulation, we modify the rheology so that icebergs are represented by thick, highly compact pieces of sea ice. These compact pieces of sea ice are held together by a modified tensile strength in the material law. In this framework, the ice mélange is considered as one single fluid, where the icebergs are realised by particles.
Using idealized test cases, we demonstrate that the proposed changes in the material law are crucial to represent icebergs with the viscous-plastic rheology. Similar to the viscous-plastic sea-ice model, the ice-mélange model is highly nonlinear. Solving the model at the resolution needed to represent the typical size of icebergs in ice mélange (< 300m) is therefore challenging. We show that the ice-mélange formulation can be approximated efficiently with a modified Newton's method. Overall, the simple extension of the viscous-plastic sea-ice model is a promising path towards the integration of ice mélange into climate models.

Modelling freezing and BioGeoChemical processes in Antarctic Sea Ice

Pathak, Raghav (1); Ricken, Tim (1); Seyedpour, Seyed Morteza (1); Thom, Andrea (1); Thoms, Silke (2); Kutschan, Bernd (2)
1: University of Stuttgart
2: Alfred Wegener Institute Bremerhaven

18:10

The Antarctic sea ice, which undergoes annual freezing and melting, plays a significant role in the global climate cycle. Since satellite observations in the Antarctic region began, 2023 saw a historically unprecedented decrease in the extent of sea ice. Further ocean warming and future environmental conditions in the Southern Ocean will influence the extent and amount of ice in the Marginal Ice Zones (MIZ), the BioGeoChemical cycles, and their interconnected relationships. The so-called pancake floes are a composition of a porous sea ice matrix with interstitial brine, nutrients, and biological communities inside the pores. The ice formation and salinity are both dependent on the ambient temperature. To realistically model these multi-phasic and multi-component coupled processes, the extended Theory of Porous Media (eTPM) presented in (Ricken, et al., 2014) is used to develop high-fidelity models capable of simulating the different seasonal variations in the region. All critical variables like salinity, ice volume fraction, and temperature, among others, are considered and have their equations of state. The phase transition phenomenon is approached through a micro-macro linking scheme. A Phase- field solidification model (Thoms, Kutschan, & Morawetz, 2014) coupled with salinity is used to model the micro-scale freezing processes and up-scaled to the macro scale eTPM model. The evolution equations for the phase field model are derived following Landau-Ginzburg order parameter gradient dynamics and mass conservation of salt. This allows for modeling the salt trapped inside the pores. For the biological part, a BioGeoChemical flux model for sea ice following (Tedesco, Vichi, & Thomas, 2012) (Vancoppenolle & Tedesco, 2017) is also set up to simulate the algal species present in the sea ice matrix. Ordinary differential equations are employed to represent the diverse environmental factors involved in the growth and loss of distinct BGC components. Processes like photosynthesis are dependent on temperature and salinity, which are derived through an ODE-PDE coupling with the eTPM model. Academic simulations and results are presented as validation for the mathematical model. These high-fidelity models will eventually lead to their incorporation into large-scale global climate models.

YRM2: New Perspectives for Model Order Reduction: Dynamical Low-rank Approximation

Organizer(s): Sulz, Dominik *(University of Tübingen)*
Kusch, Jonas *(Norwegian University of Life Sciences)*

YRM2: Dynamical low-rank approximation

Date: March 18, 2024 16:30–18:30
Room: G22/013
Chair(s): Sulz, Dominik
Kusch, Jonas

Dynamical low-rank based optimisation for computing eigenvalues in nuclear engineering

Scalone, Carmen 16:30
University of L'Aquila, Italy

The use of techniques based on dynamical low-rank approximation in eigenvalue problems, when the underlying solution has a low-rank structure, has proven to be very effective, both in the case of the rightmost eigenpairs of linear operators and in the computation of the effective eigenvalue for the neutron transport equation. In this talk, we focus on the latter problem.
In particular, we consider a previously introduced special low-rank inverse power iteration, which is very efficient in lowering memory requirements, and provide suitable rank adaptations.
We focus on a combination of the aforementioned method with techniques to optimise quantities of interest in order to obtain specific values of the effective eigenvalue. This is a joint work with L. Einkemmer and J. Kusch.

Multi-level dynamical low-rank approximation for grid-based radiation dose calculations

Stammer, Pia (1,3); Kusch, Jonas (2); Wahl, Niklas (3); Lathouwers, Danny (4) 16:50
1: Karlsruhe Institute of Technology
2: Norwegian University of Life Sciences Ås
3: German Cancer Research Centre - DKFZ
4: TU Delft

Dose predictions in radiation therapy require the solution of high-dimensional transport equations in a heterogeneous medium and with highly forward-peaked scattering. Despite the complexity of the problem, dose calculation errors of less than 2% are clinically recommended, computation times cannot exceed a few minutes and memory space on workstations is limited. This often prohibits the use of exact grid- and moment-based numerical methods.
We tackle this problem using a dynamical low-rank approach based on a multi-level collided-uncollided split, i.e., the transport equation is split through a collision source method. Uncollided particles are described using an analytical ray tracer, facilitating the use of boundary conditions and accurate physics models, including stochastic energy loss. Collided particles on the other hand, are represented using a moment method combined with the dynamical low-rank approximation. Here the energy is treated as a pseudo-time and a rank adaptive integrator is chosen to dynamically adapt the rank in energy. We find that for proton transport extremely low ranks of around r=5 are sufficient and thus computational costs and memory can be significantly reduced compared to a full-rank computation.
We then explore a generalisation of the multi-level formulation to other discretization parameters, such as an uncertainty variable or spatial and angular refinement. We discuss the optimal choice of rank or adaptation tolerance and the relation between the rank and overall error.

Multi-scale simulations of thermal radiative transfer equations using dynamical low-rank approximation

Patwardhan, Chinmay (1); Kusch, Jonas (2); Frank, Martin (1) 17:10
1: Karlsruhe Institute of Technology
2: Norwegian University of Life Sciences Ås

Phenomena like supernova explosions, star formations or radiation emitted from a hohlraum striking a fusion target, involve the formation and propagation of thermal radiation fronts called Marshak waves. Mathematically, this process can be described using the thermal radiative transfer equations, which are coupled equations governing the transport of particles and the changes in the temperature of the medium. In cases with small time scales or highly absorbing materials, the behaviour of the travelling thermal front can be well approximated by a non-linear diffusion-type equation known as the Rosseland approximation, which can be obtained as an asymptotic limit of the scaled thermal radiative transfer equations. Simulating Marshak waves using these scaled equations present several computational challenges. First, due to the high-dimensional phase space involved, substantial memory and computational resources are required. Second, to conduct multi-scale simulations, stable numerical schemes which simultaneously capture large scale dynamics as well as accurately represent the system's asymptotic behaviour are needed. To reduce computational costs we employ dynamical low-rank approximation (DLRA) which evolves a low-rank solution on a low-rank manifold and thereby significantly reduces the computational and memory requirements. Then, to drive the solution to its correct asymptotic limit, we use a macro-micro decomposition of the particle density. Combining these, we propose an asymptotic-preserving and rank-adaptive DLRA integrator for simulating Marshak waves. We show that the proposed integrator correctly discretises the Rosseland approximation in the limiting case, i.e. it is asymptotically consistent. Additionally, we show stability of the integrator in energy norm for a modal discretisaion of the linearised macro-micro system. We demonstrate the efficiency of the proposed method in a series of numerical experiments.

Projected exponential methods for stiff dynamical low-rank approximation problems

CARREL, Benjamin; VANDEREYCKEN, Bart 17:30
University of Geneva, Switzerland

The numerical integration of stiff equations is a challenging problem that needs to be approached by specialized numerical methods. Exponential integrators form a popular class of such methods since they are provably robust to stiffness and have been successfully applied to a variety of problems. The dynamical low-rank approximation is a recent technique for solving high-dimensional differential equations by means of low-rank approximations. However, the domain is lacking numerical methods for stiff equations since existing methods are either not robust-to-stiffness or have unreasonably large hidden constants.

In this talk, we focus on solving large-scale stiff matrix differential equations with a Sylvester-like structure that admit good low-rank approximations. We propose two new methods that have good convergence properties, small memory footprint and that are fast to compute. The theoretical analysis shows that the new methods have order one and two, respectively. We also propose a practical implementation based on Krylov techniques. The approximation error is analyzed, leading to a priori error bounds and, therefore, a mean for choosing the size of the Krylov space. Numerical experiments are performed on several examples, confirming the theory and showing good speedup in comparison to existing techniques.

Memory and time efficient neural network training via dynamical low-rank approximation

Schotthoefer, Steffen (1); Zangrando, Emanuele (2); Kusch, Jonas (3); Ceruti, Gianluca (4); Tudisco, Francesco (5)

1: Oak Ridge National Laboratory, USA
2: Gran Sasso Science Institute, Italy
3: Norwegian University of Life Sciences Ås
4: University of Innsbruck
5: University of Edinburgh

17:50

Neural networks have achieved tremendous success in a large variety of applications. However, their memory footprint and computational demand can render them impractical in application settings with limited hardware or energy resources. In this work, we propose a novel algorithm to find efficient low-rank subnetworks. Remarkably, these subnetworks are determined and adapted already during the training phase and the overall time and memory resources required by both training and evaluating them are significantly reduced. The main idea is to restrict the weight matrices to a low-rank manifold and to update the low-rank factors rather than the full matrix during training. To derive training updates that are restricted to the prescribed manifold, we employ techniques from dynamic model order reduction for matrix differential equations. This allows us to provide approximation, stability, and descent guarantees. Moreover, our method automatically and dynamically adapts the ranks during training to achieve the desired approximation accuracy. The efficiency of the proposed method is demonstrated through a variety of numerical experiments on fully-connected and convolutional networks.

On dynamical low-rank approximation for the Su-Olson problem

Baumann, Lena (1); Einkemmer, Lukas (2); Klingenberg, Christian (1); Kusch, Jonas (3)

1: JMU Würzburg
2: University of Innsbruck
3: Norwegian University of Life Sciences Ås

18:10

Numerically solving kinetic equations often requires a high computational effort and memory cost. One approach to tackle this difficulty is the reduced-order method dynamical low-rank approximation (DLRA). It has recently been used in various applications for an efficient and accurate numerical solution of kinetic PDEs.

In this talk, we shall apply DLRA to the thermal radiative transfer equations with Su-Olson closure. We propose a low-rank algorithm that through an implicit coupling of energy and radiation density is shown to be energy-stable. Further, we use a rank-adaptive method combined with a suitable truncation strategy to obtain conservation of mass. Numerical experiments validate the theoretical results and show the computational efficiency of the algorithm.

This is joint work together with Lukas Einkemmer, Christian Klingenberg and Jonas Kusch.

YRM3: Dynamical Systems: Discretization, model reduction and learning

Organizer(s): Cortes Garcia, Idoia *(Eindhoven University of Technology)*
Schaller, Manuel *(Technische Universität Ilmenau)*
Klioba, Katharina *(Hamburg University of Technology)*

YRM3: Dynamical Systems: Discretization, model reduction and learning

Date: March 18, 2024 16:30–18:30
Room: G22/H2
Chair(s): Cortes Garcia, Idoia
Klioba, Katharina
Schaller, Manuel

An operator-theoretic view on discretisation of random evolution equations

Klioba, Katharina; Seifert, Christian 16:30
Hamburg University of Technology

A common challenge in modelling dynamical systems consists in finding appropriate system parameters, such as diffusion coefficients. One possibility to overcome this challenge is to model them by a random variable, resulting in a random evolution equation. Since an analytical solution is typically out of reach, numerical discretisation is required.

Solving evolution equations with random coefficients numerically requires a discretisation in space, in time, and of random coefficients. Methods to treat these three problems separately are well-known, including rates of convergence. In this talk, conditions are presented under which these rates of convergence are conserved as a joint convergence rate for the fully discretised solution. Uncertainty quantification is performed by means of a polynomial chaos expansion (PCE). To illustrate this interplay of different discretisation schemes, results are discussed for the heat equation with random diffusion coefficients.

This is joint work with Christian Seifert from Hamburg University of Technology.

Dynamic Control of a Soft Robot: Combining Data and Model

Grube, Malte; Seifried, Robert 16:50
Hamburg University of Technology

Soft robots are robots made of soft materials such as silicone. They typically experience large elastic deformations. In addition, there are model uncertainties due to manufacturing inaccuracies. This makes modeling and control of soft robots challenging. As a result, most soft robots are currently limited to applications with slow motion or very low accuracy requirements. So-called kinematic controllers are used here, which, in contrast to so-called dynamic controllers, are based on a quasi-static representation of the soft robot. However, new soft robotic applications require controllers that allow more agile and precise movements. In soft robotics, open-loop control is especially important. Sensor integration is usually difficult due to the large deformations that occur and the required softness of the overall system. The model uncertainties are usually taken into account by data-driven approaches. In kinematic control, typically, inverse kinematics are learned. However, a direct extension of these approaches to dynamic control is usually not practical because the amount of training data required becomes too large. Note that in soft robotics, even for more agile applications, quasi-static behavior is typically more important than dynamics, and the quasi-static behavior is more affected by model uncertainties. This results in very different modeling requirements for the kinematic and dynamic parts of the control system.

In this contribution, the open-loop dynamic trajectory tracking control of a redundantly actuated soft robot is presented. The controller is split into a kinematic part and a dynamic part. As a kinematic controller a standard data-driven inverse kinematic control approach for soft robots is chosen. For the dynamic controller a model-based inversion is chosen. This allows an accurate representation of the inverse kinematics and a simpler representation of the dynamics to keep the amount of training

data required low. The effectiveness of this control approach for the agile trajectory tracking control of soft robots is shown in experiments.

Error bounds for Koopman-based control

Nüske, Feliks (1); Peitz, Sebastian (2); Philipp, Friedrich (3); Schaller, Manuel (3); Worthmann, Karl (3)
1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: Paderborn University
3: TU Ilmenau

17:10

Extended Dynamic Mode Decomposition (EDMD), embedded in the Koopman framework, is a widely-applied approximation technique to predict the evolution of an observable along the flow of a dynamical (control) system. In this talk, we provide finite-data error bounds for EDMD-based approximations of control-affine systems, both for (standard) EDMD with a finite dictionary and in Reproducing Kernel Hilbert Spaces. Moreover, we discuss the case of ergodic sampling (where data is obtained through a long ergodic trajectory) and i.i.d. sampling w.r.t. a chosen measure. Last, we discuss the wide applicability of these bounds for various controller designs and corresponding stability results for data-driven controllers.

Index aware learning of differential algebraic equations

Förster, Peter (1,2); Cortes Garcia, Idoia (1); Schöps, Sebastian (2); Schilders, Wil (1)
1: Eindhoven University of Technology
2: TU Darmstadt

17:30

Especially in the context of surrogate modelling, learning methods such as Gaussian process regression or neural networks can be employed to approximate the parameter dependent solution of differential equations. Their application to systems described by ordinary differential equations (ODEs) is often performed and the challenges are already known and studied. However, for systems with constraints, that is, differential algebraic equations (DAEs), additional difficulties arise that do not occur at ODE level.

In this contribution, machine learning techniques that are usually employed to learn solutions of ODEs are adapted for their application to DAEs. In particular, it focuses on the appropriate treatment and decomposition of the different types of degrees of freedom arising within DAEs. This is done by means of the dissection index, an index concept that allows for such a decomposition and for quantifiying the difficulty a given DAE conveys.

The methodology is exemplified using electric networks, though the general idea can be applied to any system of differential algebraic equations, such as, e.g., those arising in multibody dynamics.

Model reduction on manifolds: a differential geometric framework

Buchfink, Patrick (1); Glas, Silke (2); Haasdonk, Bernard (1); Unger, Benjamin (1)
1: University of Stuttgart
2: University of Twente, The Netherlands

17:50

Using nonlinear projections and preserving structure in model order reduction (MOR) are currently active research fields. In this paper, we provide a novel differential geometric framework for model reduction on smooth manifolds, which emphasizes the geometric nature of the objects involved. The crucial ingredient is the construction of an embedding for the low-dimensional submanifold and a compatible reduction map. The joint abstraction can be used to derive shared theoretical properties for different methods, such as an exact reproduction result. Moreover, it can be considered as a unifying framework for structure-preserving MOR for Lagrangian and Hamiltonian systems, MOR for transport problems, and MOR for differential-algebraic equations.

Stability and robustness in data-driven predictive control

Berberich, Julian
University of Stuttgart

18:10

While recent years have shown rapid progress of learning-based and data-driven methods to effectively utilize data for control tasks, providing rigorous theoretical guarantees for such methods is challenging and an active field of research. This talk will be about a recently developed framework for model predictive control (MPC) of unknown systems based only on input-output data which admits exactly such guarantees. The proposed approach relies on the Fundamental Lemma of Willems et al. which parametrizes trajectories of unknown linear systems using data. In this talk, we present recent findings on closed-loop guarantees of data-driven MPC with a focus on stability and robustness properties in case of noisy data or nonlinearities.

YRM4: Model Update and Parameter Identification

Organizer(s): Henkes, Alexander *(ETH Zurich)*
Wessels, Henning *(TU Braunschweig)*

YRM4: Model update and parameter identification

Date: March 18, 2024 16:30–18:30
Room: G16/H5
Chair(s): Henkes, Alexander
Wessels, Henning

Utilising Closely Spaced Modes of Tower Structures for Damage Localisation using Multi-Objective Model Updating

Ragnitz, Jasper (1); Hofmeister, Benedikt (1); Jonscher, Clemens (1); Hübler, Clemens (1,2); Rolfes, Raimund (1) 16:30

1: Leibniz University Hannover
2: TU Darmstadt

With this work, we present a multi-objective model updating approach to localise structural damage for tower structures, which possess closely spaced eigenfrequencies.
In structural health monitoring, modal quantities of structures, i.e., eigenfrequencies and mode shapes, can be used as damage sensitive features to detect and localise damage. Model updating approaches utilise these identified modal quantities to compare them to the corresponding mode shapes and eigenfrequencies of a finite element model with the aim of quantifying and minimising the discrepancy between the two by changing the local structural stiffness. The resulting modified stiffness values of the model, which fit the damaged behaviour of the real structure, can then be used to give insights into the damage location and severity.

Symmetric tower structures possess closely spaced bending modes, i.e., two bending modes have nearly the same eigenfrequency, which are often difficult to identify. Since the dominant uncertainty lies in the alignment of modes in the modal subspace, traditional methods for the comparison of two modes, such as the modal assurance criterion, are not suitable for such modes as they are susceptible to this uncertainty. Moreover, a direct comparison of the bending modes between structure and model usually yields bad results due to different mode alignments regardless of the agreement of the actual dominant vibration shapes.
To overcome this problem, the subspace of order 2 Modal Assurance Criterion (S2MAC) calculates the optimal fit between a mode shape and a subspace defined by two bending modes, thus minimising the alignment uncertainty.
Here, the basic ideas of the S2MAC are utilised and adapted to resolve the alignment issue between the mode shapes of the real structure and the model. This enables the comparison of the actual dominant vibration shapes, allowing a stable quantification of the discrepancy between model and structure based on the mode shapes.
The method is validated using an experimental girder mast structure with several reversible damage features. Acceleration sensors placed at various levels of the structure record the ambient vibrations of the structure. Mode shapes and eigenfrequencies are identified using the BayOMA method. Both are utilised for model updating by using a multi-objective deterministic algorithm to minimise the differences between the model and the measurement data. The multi-objective optimisation problem results in several Pareto-optimal solutions for the parameter identification problem.

Uncertainty quantification for two-step model calibration using least-squares and Bayesian inference

Tröger, Jendrik-Alexander (1); Römer, Ulrich (2); Hartmann, Stefan (1) 16:50
1: Clausthal University of Technology
2: TU Braunschweig

In the field of solid mechanics, constitutive models are developed to capture the material behavior of various materials, including metals, polymers, composites, glass, etc. However, to perform reliable simulations of the material response, it is crucial to determine the material parameters associated with the constitutive model from experimental data. Thus, material parameter identification or model calibration respectively is a common task in solid mechanics, typically carried out using the non-linear least-squares method. In addition to identifying the material parameters, it is essential to account for the corresponding parameter uncertainties. In this context, the field of uncertainty quantification has gained significant interest in recent years and is often linked with Bayesian methods.

This contribution deals with the two-step calibration of an elasto-plastic constitutive model using the non-linear least-squares method. Here, the calibration procedure comprises two steps. First, the elastic model response is calibrated. Subsequently, the material parameters describing the model response in the plastic domain are identified. As a novel contribution, we extend the non-linear least-squares method with an uncertainty analysis, which even takes into account the propagation of uncertainties in the step-wise procedure. Since Bayesian methods are frequently employed to compute uncertainties in model calibration applications, we follow this approach in this work as well. Finally, the uncertainties obtained by both methods - non-linear least squares and Bayesian inference - are compared under consideration of the underlying assumptions.

Probabilistic parameter identification of a rate-dependent constitutive model for porcine stomach tissue

Wollner, Maximilian P. (1); Holzer, Clarissa S. (1); Caulk, Alexander W. (2); Holzapfel, Gerhard A. (1,3) 17:10
1: University of Graz
2: Surgical, Medtronic, USA
3: Norwegian University of Science and Technology Trondheim

As computational models have grown more important for the design of medical devices and their regulatory assessment, the need for the validation and uncertainty quantification of simulations continues to increase [1].

In this work, we focus on the propagation of uncertainties from experiments, such as uniaxial tension-compression, biaxial tension-compression, and simple shear, to the constitutive model of a simple material. To define this relation between deformation history and stress state, a set of material parameters needs to be identified which is commonly achieved through a method of least squares [2]. To this end, a loss function must be minimized, the definition of which can become rather ambiguous when various multi-axial experiments are considered simultaneously. Most importantly, the method of least squares is incapable to propagate uncertainties.

These issues can be overcome by treating the calibration of constitutive models as a probabilistic problem [3]. To associate a relative likelihood to each possible set of material parameters, we derive a parameterization-invariant posterior in a Bayesian framework valid for any combination of spatially homogeneous experiments. As an application example, we calibrate a rate-dependent constitutive model at finite strains based on real data from experiments of porcine stomach tissue.

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Aspects of parameter identification in thermoplasticity

Rose, Lars (1); Menzel, Andreas (1,2)
1: TU Dortmund University
2: Lund University

17:30

Different methods and approaches for solving the inverse problem of parameter identification for various material models have been introduced in the literature within the last decades. Whether for purely mechanical models (see [1, 2, 3]), purely thermal models (see [4, 5]), or thermomechanically coupled models (see [6, 7]), taking into account different kind of underlying material effects, from fibre introduced anisotropy to damage.
The respective identification approaches are usually performed and tested under consideration of one specific material model. However, especially for thermomechanically coupled material models, different model related questions arise which are usually not mentioned in the respective publications. This talk will therefore give an overview of coupling related issues during a full field based parameter identification scheme, i.e. model related identifiability and verifiability will be discussed on the basis of two different model classes with different functional relations for the predicted dissipation rate density.
More precisely speaking, the following questions will be answered:

- What kind of data is required to guarantee identifiability of all model parameters of a thermomechanically coupled material model, including an additional, thermomechancially sound model-parameter for the scaling of dissipation?
- How do different modelling approaches influence the identifiability of the underlying parameter set?
- How do the afore mentioned modelling approaches influence the verifiability of the respective models (for a specific, real material)?

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Optimization of the specimen geometry for one-shot discovery of material models

Ghouli, Saeid (1); Flaschel, Moritz (2); Kumar, Siddhant (3); De Lorenzis, Laura (1) 17:50
1: ETH Zurich
2: Weierstrass Institute for Applied Analysis and Stochastics
3: TU Delft

We recently proposed an approach for Efficient Unsupervised Constitutive Law Identification and Discovery (EUCLID), which exploits machine learning tools such as sparse regression [1–3], Bayesian learning [4], or neural networks [5] to automatically discover material laws independent of stress data, but solely based on full-field displacement and global force data obtained from mechanical testing. The displacement field can be measured on the surface of a target specimen via digital image correlation (DIC).

An important feature of the approach is that, in principle, the discovery of the material law can be performed in a one-shot fashion, i.e., using only one experiment. However, this capability heavily relies upon the richness of the measured displacement data, i.e., their ability to probe the stress-strain space (where the stresses depend on the constitutive law being sought) to an extent sufficient for an accurate and robust discovery process. The richness of the displacement data and the robustness of the discovery process are in turn governed by the specimen geometry.

In the present study, we aim to optimally design the geometry of the target specimen via density-based topology optimisation approach. In this fashion, we perform automatic specimen design by maximising the robustness of the solution, i.e., the identified material parameters, given noisy displacement measurements from DIC. In this contribution, we shed light on the objective function, the topology optimisation framework, and a range of optimised topologies for orthotropic elasticity.

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An extension of the Dynamic Regressor Extension and Mixing approach for real-time parameter estimation

Othmane, Amine 18:10
Saarland University

Numerical values of model parameters are often not or only poorly known and must be inferred from measurements. Estimation problems can often be formulated as linear regressions, which can be solved using gradient-descent or least squares estimators. The convergence of these approaches relies on the persistency of excitation of the regressor, which is a restrictive condition, and the transient performance of these estimators is challenging to analyze. Dynamic Regressor Extension and Mixing has recently been proposed as a new method for system identification and adaptive control. Its convergence does not rely on the persistency of excitation condition of the regressor. The main idea is to generate as many new independent linear regression equations as there are parameters to be estimated. Nonlinear manipulations of the data and a gradient-descent estimator then guarantee that the estimation error of each parameter satisfies an independent differential equation.

The generation of new independent equations required in this method is analyzed in this contribution using orthogonal projection operators. The latter have beneficial robustness properties regarding perturbed measurements. Linear time-varying observers using these operators are proposed to estimate piecewise constant parameters. They require weaker conditions for the estimation errors to converge to zero compared to known approaches. An important property is that parameters are continuously adapted, even if some are not or only poorly excited on arbitrary time intervals. The approaches are validated in simulations and experiments with perturbed measurements.

YRM5: Computational Mechanics of Active Biological Systems

Organizer(s): Brandstäter, Sebastian *(University of the Bundeswehr Munich)*
Lambers, Lena *(University of Stuttgart)*

YRM5: Computational Mechanics of Active Biological Systems

Date: March 18, 2024 16:30–18:30
Room: G26/H1
Chair(s): Lambers, Lena
Brandstäter, Sebastian

Aneurysm treatment: About in silico device insertion, a porous media surrogate and LBM Bloodflow simulations

Holzberger, Fabian; Horvat, Medeea; Lunowa, Stephan; Nebulishvili, Natalia; Muhr, Markus; Sytnyk, Dmytro; Wohlmuth, Barbara 16:30
Technical University of Munich

Cerebral Aneurysms are pathological outpouches of bloodvessels in the brain resulting e.g. from structural weakening of the arterial wall. Aneurysm rupture resp. the resulting stroke is a creeping danger to patients with high mortality and morbidity rate in Western civilization. It is hence of importance to better understand factors influencing the rupture risk, as well as assessing the chances of success vs. aneuryms-recurrence for different treatment-methods on short- and longterm timelines. Ultimately it is our goal within the *SPP 2311 project* to develop a clinical surgeon's tool for simulation-based, patient-specific aneurysm treatment optimization.

In this talk, we present Lattice-Boltzmann-method based research and simulation results regarding bloodflow within realistic, 3D and patientspecific vessel- and aneurysm-geometries reconstructed from angiography-scans. Starting from this ***preoperative state***, a risk-assessment w.r.t. the risk of rupture of the aneurysm can be performed based on quantities of interest (QoIs) such as the wall-shear-stress.

Subsequently we are interested in the in-silico ***simulation of the corresponding medical treatment*** by means of insertion of endovascular treatment devices. Depending on the type of aneurysm, we incorporate stents, flow-diverters and Woven-Endo-Bridge-devices by means of geometrical models as well as the procedure of endovascular coiling by a 3D-embedded mechanical 1D-wire insertion simulation. The mechanical model takes into account manufacturer-predefined micro-structures giving the coil its characteristic mechanical curling-behaviour.

After insertion again the hemodynamics, now within the treated aneurysm, are considered in order to evaluate how the device influences flow-characteristics and rupture-relevant QoIs. These bloodflow-simulations are either conducted in a fully resolved (DNS) fashion or by means of a porous medium surrogate model for the endovascular device, where the porous field parameters are obtained via an averaging procedure from the actual device's geometry. Within this ***postoperative state*** questions regarding the occlusion quality of certain types of devices or factors increasing the risk of re-growth/recurrence of the aneurysm due to insufficient occlusion are discussed.

In terms of ***long-term prognosis*** of the treatment outcome further bio-active components such as the formation and growth of a thrombus between the medical device's wires are of interest. On the one hand, thrombosis is wanted and does increase the aneurysm occlusion-ratio, while on the other hand, excessive blood-clotting might also result in additional risks such as stenosis. Furthermore also the incorporation of aneurysm-wall (weakening) effects, due to bloodstream pulsation, or the formation of an edema in the (brain) tissue outside the aneurysm are goals of the project.

Microstructure-informed regional constitutive modeling of human brain tissue

Reiter, Nina; Bräuer, Lars; Paulsen, Friedrich; Budday, Silvia
FAU Erlangen-Nürnberg

16:50

Continuum-mechanics based computational models of the human brain can help to better understand mechanics-related processes of neurodevelopment, injury, and disease. A major challenge is, however, that brain tissue is extremely complex both on the microscopic and macroscopic scale: on the microscale, it is challenging to identify load-bearing structures since brain tissue does not contain fibrous collagen like many other tissues; on the macroscale, the brain is divided into many anatomical regions that strongly differ in their microstructural organization and mechanical response.

In a recent study, we have shown that considering the differences of those anatomical regions is essential to ensure the accuracy of whole-brain simulations [1]. However, calibrating material parameters for multiple brain regions remains a challenge: in phenomenological material models, the calibrated parameters are often highly sensitive to experimental boundary conditions and cannot be transferred to tissues that differ from the ones used for calibration. This issue can be overcome with microstructure-motivated material models that have microstructural parameters with a physical meaning. Such parameters could be adapted to account for differences between individuals or changes associated with aging or neurological disease. Here, we correlate mechanical data from multimodal, large-strain experiments on healthy, postmortem human brain tissue with microstructural data of the same samples from histological examination as a first step towards microstructure-informed constitutive models for different anatomical regions of the human brain. Additionally, we consider observations from multiscale experiments with simultaneous mechanical testing and microstructural observation that shed light on the role of axons and blood vessels during brain deformation [2]. Taken together, these insights lay the groundwork for fully microstructure-based material models for human brain tissue.

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Modelling muscle-actuated motion: Benefits for internal mechanics, optimization and learning

Wochner, Isabell (1); Schmitt, Syn (2); Haeufle, Daniel (1)
1: Heidelberg University
2: University of Stuttgart

17:10

Humans have the remarkable ability to effortlessly perform and learn complex and versatile movements whether walking through uneven terrain, lifting and manipulating objects or playing sports. These abilities are the result of the intricate interplay between our neural control system, the underlying musculoskeletal system and the environment. Hence, understanding the mechanics governing muscle-driven motion is crucial. However, despite extensive research, the neural control of muscle-actuated motion remains elusive also due to limitations in experimental approaches.

Simulations of muscle-driven motion have emerged as a vital tool to overcome ethical and practical constraints, allowing us to uncover cause-effect relationships which cannot be measured experimentally. Such simulations enable us to change morphological aspects of the musculoskeletal structure or the neural control strategy, yielding crucial insights into muscle-driven motion mechanics.

The insights hold promise for advancing rehabilitation techniques, refining surgical planning, innovating assistive devices, and enhancing the performance of existing robots.

In this talk, I will show that muscle-tendon dynamics are beneficial for controlling and learning biological movements. To do so, both model-based and learning-based methods (including optimal control,

model predictive control and reinforcement learning) are used to control biological and robotic models. Based on my work, I show that it is crucial to include muscle dynamics to (1) correctly predict voluntary movements, (2) simplify the control in terms of morphological computation, and (3) use the inherent benefits of muscles to learn robust motions more data-efficiently.

Modelling of micro crack healing in flexoelectric bones

Witt, Carina (1); Kaiser, Tobias (1); Menzel, Andreas (1,2)
1: TU Dortmund University
2: Lund University

17:30

Micro cracks, which naturally occur in bones under mechanical loading, are successively healed by a process called bone remodelling under the activity of different types of bone cells. The main cell types involved are osteoclasts and osteoblasts which are responsible for the resorption of old bone as well as the formation of new bone material, respectively. However, osteocytes play an even more important role in the process since they initiate bone remodelling by signalling mechanisms. This initiation is attributed to different phenomena in the literature which are closely related to electromechanical coupling. One particular mechanism that was experimentally observed in cortical bone between 2018 and 2020 [1,2] is flexoelectricity – i.e. the coupling between strain gradients and electric polarisation. Since large strain gradients occur in the vicinity of cracks in response to mechanical load, this effect is considered to be particularly relevant in the context of crack healing and, especially, for micro cracks due to its size-dependency.
In the present contribution, the process of targeted remodelling in cortical bone is investigated via a computational framework. Due to the higher-order characteristic of flexoelectricity, Isogeometric Analysis is employed to resolve the flexoelectric initiation of the process whereas the subsequent bone cell diffusion as well as the resulting crack healing is accounted for in a classic Finite Element framework. The latter is combined with a surface growth algorithm in which the finite element mesh is updated in each growth step in order to incorporate the production of bone material. By the example of a micro-sized bone sample with a narrow micro crack, it is shown that the proposed framework is capable of representing the whole process of bone remodelling, based on flexoelectric initiation. Therein, anisotropy is considered for both the bone structure as well as for the diffusion tensors of the bone cell concentrations. These concentrations are accounted for as independent fields and interact with each other through different mechanisms such as source terms and boundary conditions. The presented work is based on the model proposed in [3] and extended with regard to surface growth and the modelling of the diffusion processes.

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Stabilized Finite Element Simulation to Determine Washout in The Left Ventricle with Implanted Left Ventricular Assist Device

Schuster, Maximilian Roman; Hosters, Norbert; Behr, Marek
RWTH Aachen University

17:50

Left ventricular assist devices (LVADs) play an important role in helping patients with heart disease, primarily as a bridge to transplantation [1]. We simulate the interaction between blood flow in the left ventricle, the LVAD flow rate, and the cannula inserted into the ventricle. To reduce complications such as thrombosis, it is important to study blood flow in the left ventricle under LVAD support. We identify areas of stagnation by solving transport equations for the Virtual Ink method in the ventricle under different LVAD operating conditions. Such areas of stagnation and low velocity are prone to thrombosis.

From the point of view of computational mechanics, the definition of appropriate boundary conditions plays a crucial role in this project for the structural and fluid mechanics parts, respectively. The fluid boundary conditions at the valves and the LVAD cannula are obtained from a 0D lumped parameter network of the cardiovascular system. The interaction between the ventricular wall and the fluid is imposed by the wall motion. In our current work, we use a magnetic resonance imaging (MRI) based left ventricular geometry and interpolate the ventricular mesh motion with radial basis functions. The LVAD cannula is implanted at the apex and the pump flux is set as a time-dependent Dirichlet boundary condition.

An in-house code [2] is used for the different stages of the simulation. It uses a stabilised finite element method to discretise time and space. The fluid is subject to the incompressible Navier- Stokes equations with a Newtonian material law. The key result is washout as a function of the LVAD operating conditions.

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Constitutive modeling of active skeletal muscle in a continuum-mechanical model of the human shoulder

Engelhardt, Laura; Sachse, Renate; Burgkart, Rainer; Wall, Wolfgang A. 18:10
Technical University of Munich

The human shoulder joint combines mobility and stability in a unique musculoskeletal system. The anatomical structure of the glenohumeral joint allows for an extensive range of motion, while passive and active soft tissues ensure the joint's integrity through static and dynamic mechanisms.

Maintaining this delicate balance between mobility and stability is essential for proper shoulder function, yet it is easily disrupted by injury or pathological conditions. Despite the high incidence of shoulder disorders in clinical practice, understanding of the underlying biomechanics remains limited, posing major challenges for medical assessment and treatment.

Computational musculoskeletal models offer great potential for biomechanical studies of the shoulder's physiology, investigations of pathological conditions, objective predictions and evaluations of (patient-specific) treatments, and the development of rehabilitation equipment for physical therapy.

While numerous reduced-dimensional multi-body models exist, research on comprehensive continuum-based finite element models remains limited. However, three-dimensional interactions between the joint components, such as contact and sliding mechanisms, are central to the shoulder's physiology. In contrast to multi-body models, continuum-mechanical models can represent such volumetric effects, account for complex muscle fiber and tendon arrangements, and model sophisticated constitutive behavior.

Considering their role as active joint stabilizers and force generators, skeletal muscles deserve special attention regarding their material description. Passive skeletal muscle is - according to its histological composition - commonly modeled as a transverse isotropic composite of unidirectionally oriented fibers connected by extracellular tissue. Active contractile effects are incorporated through active-stress or (generalized) active-strain approaches. Since selecting an appropriate constitutive model is crucial for reliable predictions, the question arises of which material is best suitable for characterizing the shoulder's skeletal muscles.

In this contribution, we contrast three hyperelastic formulations considering mathematical, computational, and physiological aspects: an active-stress, an active-strain, and a generalized active-strain approach.

We discuss the concepts of modeling active material behavior from a mathematical and physiological perspective, address analytical and numerical problems arising from the mathematical formulations, and analyze the included biophysical principles of force generation in terms of physiological correctness and relevance considering the modeling of the human shoulder. Conclusively, we present a constitutive model combining the studied materials' most promising and relevant properties. By the example of a fusiform muscle geometry, we investigate force generation, deformation, and kinematics during active isometric and free contractions. Eventually, we demonstrate the applicability of the material formulations in simulations of a comprehensive continuum-mechanical model of the human shoulder.

DFG Programs

GRK 2297: Mathematical Complexity Reduction

Organizer(s): Sager, Sebastian *(Otto-von-Guericke Universität Magdeburg)*

DFG-GRK 2297: Research Training Group Mathematical Complexity Reduction

Date: March 19, 2024 14:00–16:00
Room: G22/020
Chair(s): Heiland, Jan
Nüske, Feliks
Richter, Thomas

Bi-linear Control Based On gEDMD for Metastable Systems

Guo, Lei; Nüske, Feliks; Heiland, Jan 14:00
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Stochastic systems influenced by an external affine control input are an interesting approach towards understanding the dynamics of complex metastable systems. External input can accelerate transition from state around local minimum to another one with significantly reduced time. Such stochastic differential systems can be identified by a data-driven method, which is an extension of Extended Dynamic Mode Decomposition, called generator-EDMD and introduced in [Klus et al. (2020)]. This method has been successfully used to approximate the Koopman generator of stochastic systems. Koopman generators, for the stochastic differential systems with an affine control input, transform the kolmogorov backward equation into ordinary differential equation that is bilinear in expectation and input, and this structure can be leveraged for the design of controllers and the prediction of the expected values in the finite-dimensional subspace. We numerically apply gEDMD to predict the expectations of one-dimensional overdamped langevin dynamics with double-well potential.

Smooth clustering-based autoencoders for very low-dimensional parametrizations of fluid flow models

Heiland, Jan (1,2); Kim, Yongho (1,2) 14:20
1: Otto von Guericke University Magdeburg
2: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Model order reduction techniques have been developed to decrease the computational complexity of large-scale systems while maintaining a certain accuracy. One standard way is to utilize proper orthogonal decomposition (POD) to build reduced order models. POD is the method of choice owing to its linearity, the orthogonality of POD modes, and its optimality as a linear projection. Nevertheless, the linear nature of POD comes to a limit for state reconstruction when applied to nonlinear dynamical systems with very reduced order dimensions. As an alternative, nonlinear autoencoders (AEs) have been widely used due to their nonlinearity and compatibility with other machine learning methods, thereby enhancing reconstruction performance. In this work, we introduce clustering-based autoencoders for very low-dimensional parametrizations of fluid flow models. However, this approach is

not suitable for dynamical systems derived from partial differential equations due to the discontinuity inherent in many clustering algorithms including k-means clustering. Therefore, we discuss how to maintain continuity by the integration of autoencoders and differentiable clustering networks and evaluate this new approach in numerical simulations.

Physics-based, non-intrusive modeling for systems with spatially localized behavior through reduced/full-order model coupling

Gkimisis, Leonidas (1); Aretz, Nicole (3); Tezzele, Marco (3); Benner, Peter (1,2); Richter, Thomas (2); Willcox, Karen E. (3)

1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: Otto von Guericke University Magdeburg
3: The University of Texas at Austin, USA

14:40

Physics-based, non-intrusive modeling comprises a promising solution to dynamics prediction for systems with partially known physical laws, for which data are available, either through experimental campaigns or proprietary software simulations. Non-intrusive, reduced-order modeling methods are specifically interesting, as they allow for high computational efficiency by projecting the system dynamics onto a basis of reduced dimension. The inferred reduced-order models are highly accurate for a wide class of dynamical systems. From a different perspective, a recent line of work has focused on the inference of phyiscs-informed, full-order models (FOMs) which govern system dynamics. This approach is motivated by the sparsity of polynomial operators in spatially discretized partial differential equations. Exploiting sparsity creates the potential for computation and storage of otherwise intractable, non-intrusive FOMs. Under this perspective, inferred models are independent of a projection basis, which could in turn allow for dynamical predictions beyond the span of the training data. Nonetheless, this capability comes at a significant offline and online computational cost. In this work we investigate the potential of leveraging the capabilities of localized, sparse FOM inference with the high computational efficiency of a non-intrusive ROM, via domain decomposition for systems with localized, slow singular value decay. Assuming state access, the spatial domain is decomposed into two subdomains where the system dynamics exhibit slow and fast singular value decay, respectively. By inferring a full-order model on the former subdomain, we aspire to capture phenomena with slow singular value decay, such as advection-dominated dynamics. Employing a ROM for the latter subdomain considerably restricts the involved computational cost for the overall system inference, while retaining prediction accuracy over the span of the training data. Approaches for deriving the coupled, domain-decomposed, non-intrusive FOM/ROM system are being discussed. Finally, we present numerical results for linear and nonlinear systems which arise in fluid dynamics problems.

Error analysis for hybrid finite element/neural network discretizations

Kapustsin, Uladzislau; Kaya, Utku; Richter, Thomas

Otto von Guericke University Magdeburg

15:00

In this talk we present a hybrid finite element/neural network method for predicting solutions of partial differential equations. The method is designed for obtaining fine scale corrections for the coarse solutions from neural networks in a local manner. The network is capable of locally correcting a coarse finite element solution towards a fine solution by taking the local values of the coarse approximation as well as other local information like values of the source term or velocity field as input. The key observations is the dependency between quality of predictions and the size of training set which consists of a set of different problems, e.g. with different source terms or velocity fields, and corresponding fine and coarse solutions. We provide the a priori error analysis of the method together with the stability analysis of the neural network. To support the theoretical claims we present the results of the numerical experiments. We also illustrate the generalization of the method to problems where test and training problems differ from each other, for instance in terms of domain, time, source terms, etc.

Source Detection on Graphs

Feldmann, Sarah; Sager, Sebastian; Kaibel, Volker 15:20
Otto von Guericke University Magdeburg

The source detection problem consists of a weighted connected graph and a signal spreading through it with the following properties. The signal is sent with a constant velocity from a unique unknown source node. For each node there is the possibility to measure the time at which the signal reaches the node. The goal is to find the source node with as few measurements as possible without knowledge of the starting time or the velocity of the signal. This talk takes two cases into account. In the deterministic offline case I introduce the combinatorial concept of the spread dimension. Assuming exact computation and no measurement errors, the objective is to determine as few as possible measurement nodes to uniquely locate the source node, no matter which node actually turns out to be the source. In the stochastic online case it is discussed how to find a probable source with an iterative algorithm using parameter estimation and experimental design. This iterative approach requires a repetitive nature of the signal so that in each iteration the information gained in the previous iterations can be used.

Refined TSSOS

Shaydurova, Daria; Kaibel, Volker; Sager, Sebastian 15:40
Otto von Guericke University Magdeburg

The moment-sum of squares hierarchy by Lasserre has become an established technique for solving polynomial optimization problems. It provides a monotonically increasing series of tight bounds, but has well-known scalability limitations. For structured optimization problems, the term-sparsity SOS (TSSOS) approach scales much better due to block-diagonal matrices, obtained by completing the connected components of adjacency graphs. This block structure can be exploited by semidefinite programming solvers, for which the overall runtime then depends heavily on the size of the largest block. However, already the first step of the TSSOS hierarchy may result in large diagonal blocks. We suggest a new approach that refines TSSOS iterations using combinatorial optimization and results in block-diagonal matrices with reduced maximum block sizes. Numerical results on a benchmark library show the large potential for computational speedup for unconstrained and constrained polynomial optimization, while obtaining almost identical bounds in comparison to established methods.

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

Organizer(s): Dolzmann, Georg *(Universität Regensburg)*

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

Date: March 19, 2024 14:00–16:00
Room: G22/H2
Chair(s): Dolzmann, Georg

On the homogenization into generalized continua: a computational approach for parameter identification for the Relaxed Micromorphic Model

Scheunemann, Lisa (1); Sarhil, Mohammad (1,2); Schröder, Jörg (2); Neff, Patrizio (2) 14:00
1: RPTU Kaiserslautern-Landau
2: University of Duisburg-Essen

The relaxed micromorphic model [1] has demonstrated many advantages over other higher-order continua. Bounded from above and below, it establishes two distinct scales governed by standard linear elasticity with micro and macro elasticity tensors. Operating as a two-scale elasticity model, a characteristic length regulates the transition (size-effects) while maintaining the scale-independence of other parameters. However, identifying material parameters for enriched continua remains an ongoing research challenge, entailing difficulties such as defining a representative volume element and selecting appropriate boundary conditions to induce specific deformation modes.

In our talk, we present our recent findings in identifying the material parameters and boundary conditions in the relaxed micromorphic model [2,3], furthermore a novel numerical homogenization approach will be introduced which avoids the classical macro-micro transition approach.

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[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. Computational Mechanics **72**, 1091–1113 (2023).

Reinterpreting laminate composite voxels in computational micromechanics: level sets and assumed strain methods

Lendvai, Jonas; Schneider, Matti 14:20
University of Duisburg-Essen

The composite voxel method [1,2] permits to accelerate FFT-based computational methods by providing a substitute constitutive law for heterogeneous voxels. In fact, such heterogeneous voxels arise when coarsening a fine voxel grid or whenever the microstructure is given analytically. Subsequent works [3–5] provided strategies for general inelastic and finite strain mechanics, suggesting a more fundamental reason for the success of composite voxel technologies.

We present a natural derivation of the laminate composite voxel technique as an assumed strain method, i.e., the general framework introduced by Simo-Rifai [6], for a specific choice of the extended strain field. Therefore, laminate composite voxels arise from a kinematic assumption within a discretization scheme instead of a judiciously constructed constutive law, as originally assumed.

Moreover, we propose a straightforward way to integrate composite voxels into a given level-set framework for describing heterogeneous microstructures. We focus on the efficiency and accuracy of computing normals and cut-volume fractions of composite voxels within this framework.

References

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Co-Design of variational formulations and par- allel solvers in Non-Isothermal Thermo-Chemo- Mechanics: Comparison of Minimization and Saddle- Point formulation and scalability studies

Kiefer, Bjoern; Prüger, Stefan; Rheinbach, Oliver; Röver, Friederike 14:40
TU Bergakademie Freiberg

Mathematically sound models and efficient solution procedures for thermo-chemo-mechanical boundary value problems have gained increasing interest over the past decades, as the simulation of these coupled multi-field problems forms an integral part in understanding processes like frontal polymerization in 3D-printing, microstructure evolution in Li-ion batteries and embrittlement of steel due to hydrogen diffusion. In this contribution, the fully coupled deformation-diffusion boundary value problem of a swelling hydrogel is considered as it is a well understood benchmark problem [L. Boeger, et al., Int. J. Solids Struct., 121, 2017], to compare different finite element implementations emerging from the formulation of the rate-type variational problem as a minimization and a saddle-point problem. Besides the illustration of advantages and disadvantages of the two competing formulations in terms of e.g. matrix structure, convergence; results of scalability studies are also presented that are based on a seamlessly integrated parallel solver framework [B. Kiefer, et al., Comput. Mech., 71, 2023] using the finite element library deal.II and the parallel implementation of the FROSch (Fast and Robust Overlapping Schwarz) solver framework of the Trilinos software library. The FROSch solver employs the GDSW domain decomposition preconditioner and allows a fully algebraic construction and, in its basic form, therefore does not require geometric information. Strong scaling results up to 4000 cores are presented for representative examples of the coupled deformation-diffusion problem.

Phase transformation in elasto-plastic materials - a multi-phase simulation

Dinkelacker-Steinhoff, Sarah; Hackl, Klaus 15:00
Ruhr University Bochum

The evolution of microstructures can be observed in various engineering and natural materials, such as special alloys, silica glasses or soils. These macroscopic and microscopic effects are often controlled by thermal and chemical changes or extern forces. In addition, serveral phases are usually involved in these processes, whose energy potentials result in a non-convex total energy. A theory is presented that can be applied to a wide range of elasto-plastic materials with kinematic hardening. In order to obtain a general model, a relaxed free energy in small strain theory is defined using variational

principles for inelastic materials. This energy includes the dissipation of the substance as so-called dissipation distances to facilitate a time-stepped incremental representation. Furthermore, the phase volume fractions are contained in the weighted sum of the individual energies and are expressed here using young measures. In the centre of the model, transition rates with underlying ordinary differential equations (ODEs) are calculated, which allow access to the phase evolution of the system. The initial results and the behaviour of this theory are explained using numerical simulations created with the programming language Julia.

Structure-preserving approximation for quantitative variational phase-field models in the context of powder-bed fusion additive manufacturing

Brunk, Aaron (1); Egger, Herbert (2); Habrich, Oliver (2,3); Oyedeji, Timileyin (4); Schumann, Dennis (1); Xu, Bai-Xiang (4)

1: Johannes Gutenberg University Mainz
2: Johannes Kepler University Linz, Austria
3: Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria
4: TU Darmstadt

15:20

Powder Bed Fusion (PBF) is an additive manufacturing (AM) process, in which metallic objects are assembled layer-by-layer by selective melting of metallic powder through laser or electron beams. The complexity of the underlying physical processes impedes the thorough understanding of all the relevant phenomena involved and complicates the control and reproducibility of the production process.

To improve the understanding of the above processes we consider a quantitative phase-field model, based on basic laws of thermodynamics, to model the complex phenomena and arsing interfaces in the production process.
To simulate the different aspects encoded in the model we propose and analyse
a so-called structure-preserving method, i.e. we construct the method such that the laws of thermodynamics which are encoded in the equations are preserved hold even for the discrete approximations. This leads to robust and stable methods for which we can transparently perform the error analysis by using relative entropy type methods.

Mapping Shear Transformation Zones in Silica Network Glass

Shekh Alshabab, Somar; Wu, Zhao; Markert, Bernd; Bamer, Franz

RWTH Aachen University

15:40

The presence of long-range disorder and the lack of clearly defined defect regions makes understanding the behavior of glasses on the nano-scale challenging. However, according to shear transformation zone (STZ) theory, weak spots prone to plastic rearrangements exist and can be identified in the stress-free configuration. Various predictive methods, such as energy approximations and local structural indicators, have been proposed to varying degrees of success. However, leveraging deep mechanical insights, the local yield stress (LYS) method has shown promising success in the a priori prediction of these spots. Employing the LYS method, we identify and analyze the distribution of the weak spots in vitreous silica network glass samples, which have been generated by the Monte-Carlo bond switch algorithm and subsequently subjected to true shear using AQS. The MC algorithm allows us to generate systems with different levels of heterogeneity to study the disorder's impact on the predictability of these spots. Furthermore, we determine the average spot size by optimizing the free radius across multiple samples and investigating its relationship with the heterogeneity. Intriguingly, our results indicate an improvement in prediction accuracy with increased heterogeneity, alongside a decrease in the optimal spot size.

SPP 2298: Theoretical Foundations of Deep Learning

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

DFG-PP 2298: Theoretical Foundations of Deep Learning

Date: March 19, 2024 14:00–16:00
Room: G22/013
Chair(s): Thesing, Laura
Kutyniok, Gitta

Foundations of Supervised Deep Learning for Inverse Problems

Auras, Alexander (1); Burger, Martin (2,3); Kabri, Samira (2); Möller, Michael (1)
1: University of Siegen
2: Helmholtz Imaging, Deutsches Elektronen-Synchrotron DESY
3: Universität Hamburg

14:00

The aim of this talk is to present the work and findings of the project 'Foundations of Supervised Deep Learning for Inverse Problems'. We propose a framework to analyze data-driven reconstruction operators for inverse problems, based on the classical theory of convergent regularizations and illustrate this concept with several approaches to train a linear spectral regularizer. To draw a connection to approaches that use plug and play priors, we further present a-priori rules to simulate noise in the training process, meaning that the choice of training noise only depends on the noise level. Lastly, we investigate ways to develop theoretically founded approaches to learn reconstruction operators that go beyond linear regularization, for example by using input-invex architectures to parametrize the regularization functional.

Combinatorial and implicit views on parameter optimization in neural networks

Montufar, Guido (1,2)
1: University of California, Los Angeles, USA
2: Max Planck Institute for Mathematics in the Sciences

14:20

I discuss parameter optimization in neural networks with a view on combinatorial structures in parameter space which highlight the role of the training data and the set of feasible predictions parametrized by the network. For regression with ReLU networks I present results showing in various cases that mild overparametrization is sufficient to ensure that most regions of the parameter space associated with different activation patterns of the units over the training data have no bad differentiable critical points. Turning to classification, I present some results on the error surface and the solution sets depending on the training data. The talk is based on joint works with Kedar Karhadkar, Michael Murray, Hanna Tseran, Marie Brandenburg, Georg Loho.

Regularized, structure-preserving neural networks for the minimal entropy closure of the Boltzmann moment system

Schotthoefer, Steffen (1); Laiu, Paul (1); Hauck, Cory (1); Frank, Martin (2)
1: Oak Ridge National Laboratory, USA
2: Karlsruhe Institute of Technology

14:40

The main challenge of large-scale numerical simulation of radiation transport is the high memory and computation time requirements of discretization methods for kinetic equations. In this work, we derive an approximation to the entropy closure method to accurately compute the solution of the multi-dimensional moment system with a low memory footprint and competitive computational time. We extend structure-preserving, neural network-based approximations of the closure of the moment system to the context of regularized entropy closures. The main idea is to interpret structure-preserving neural network approximations of the regularized entropy closure as a two-stage approximation to the original entropy closure. We conduct a numerical analysis of this approximation and investigate optimal parameter choices. Our numerical experiments demonstrate that the method has a much

lower memory footprint than traditional methods with competitive computation times and simulation accuracy.

Adaptive Step Sizes for Preconditioned Stochastic Gradient Descent
Köhne, Frederik (1); Kreis, Leonie (2); Schiela, Anton (1); Herzog, Roland (2)
1: University of Bayreuth
2: Heidelberg University
15:00

The choice of the step size (or learning rate) in stochastic optimization algorithms, such as stochastic gradient descent, plays a central role in the training of machine learning models. Both theoretical investigations and empirical analyses emphasize that an optimal step size not only requires taking into account the nonlinearity of the underlying problem, but also relies on accounting for the local variance within the search directions. In this presentation, we introduce a novel method capable of estimating these fundamental quantities and subsequently using these estimates to derive an adaptive step size for stochastic gradient descent. Our proposed approach leads to a nearly hyperparameter-free variant of stochastic gradient descent. We provide theoretical convergence analyses in the special case of stochastic quadratic, strongly convex problems. In addition, we perform numerical experiments focusing on classical image classification tasks. Remarkably, our algorithm exhibits truly problem-adaptive behavior when applied to these problems that exceed theoretical boundaries. Moreover, our framework facilitates the potential incorporation of a preconditioner, thereby enabling the implementation of adaptive step sizes for stochastic second-order optimization methods.

Non-vacuous PAC-Bayes bounds for Models under Adversarial Corruptions
Mustafa, Waleed; Liznerski, Philipp; Ledent, Antoine; Wagner, Dennis; Wang, Puyu; Kloft, Marius
RPTU Kaiserslautern-Landau
15:20

PAC-Bayes generalization bounds have been shown to provide non-vacuous performance certificates for several Machine Learning models.However, under adversarial corruptions, these bounds often fail to maintain their non-vacuous nature due to the increased empirical risk. In this work, we address this limitation by deriving
and computing the first non-vacuous generalization bounds for models operating under adversarial conditions. Our approach combines the PAC-Bayes and Adversarial Smoothing frameworks to derive generalization bounds for randomly smoothed models. We empirically demonstrate the efficacy of our bounds in providing robust population risk certificates for stochastic Convolution Neural Networks (CNN) operating under L2 -bounded adversarial corruptions for both MNIST and CIFAR-10.

Convergence results for gradient flow and gradient descent systems in artificial neural network training
Ahmadova, Arzu
University of Duisburg-Essen
15:40

The realm of artificial neural network (ANN) training has witnessed considerable interest in recent years, prompting researchers to delve into diverse mathematical approaches to refine the training process. ANNs have seen growing application in tasks like image recognition, speech recognition, and natural language processing (NLP) owing to their capacity to grasp intricate and abstract patterns from vast datasets.

This paper specifically directs its attention toward elevating the existing comprehension of gradient flow and gradient descent optimization methodologies. Our primary objective is to establish a robust mathematical convergence theory concerning:

- Continuous-time gradient flow (GF) equations
- Gradient descent (GD) dynamics

SPP 2311: Robust Coupling of Continuum-Biomechanical in Silico Models to establish active biological System Models for later use in clinical Applications - Co-design of Modeling, Numerics and Usability

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

DFG-PP 2311: Robust coupling of continuum-biomechanical in sili-co models to establish active biological system models for later use in clinical applications - Co-design of modeling, numerics and usability

Date: March 19, 2024 14:00–16:00
Room: G16/H5
Chair(s): Ricken, Tim
Röhrle, Oliver
Budday, Silvia

Comparison of Pericardium Modeling Approaches for Mechanical Whole Heart Simulations

Krauß, Jonathan; Gerach, Tobias; Stengel, Laura; Wieners, Christian; Loewe, Axel 14:00
Karlsruhe Institute of Technology

The human heart sits inside the thoracic cavity and is enclosed in the pericardial sac (or pericardium). The pericardium restricts the cardiac motion during the heart cycle but allows for frictionless sliding along its inner surface. The restraining effect of the pericardium and surrounding tissues on the human heart is essential to reproduce physiological valve plane movement in simulations and can be modeled in different ways.

In this study, we investigate five different approaches used in recent publications and apply them to the same whole heart geometry. Some approaches use Robin boundary conditions, others use a volumetric representation of the pericardium and solve a contact problem (sliding contact formulation). These two strategies are combined with a smooth spatially varying scaling or a region-wise partitioning of the epicardial surface. We investigate the effect of the modeling choice on left ventricular twist (no MRI data available), stroke volume, as well as the displacement of the mitral and the tricuspid valve and compare the results to MRI cine data of the same patient. Additionally, we analyze simulation times as well as contact pressures and contact distances for all scenarios.

In general, all scenarios follow the same morphology regarding mitral valve displacement, tricuspid valve displacement and left ventricular twist. We show that – with the parameters used in the original papers – Robin boundary conditions are computationally more expensive and lead to smaller stroke volumes and less ventricular twist. Unrelated to this, simulations with a penalty scaling result in a less pronounced displacement of the tricuspid valve.

Reduced twist for the scenarios with Robin boundary conditions can be explained by the fact that Robin boundary conditions are only valid for small rotations of the epicardial surface. Higher computational times for the simulations using Robin boundary conditions are a direct result of the increased number of iterations the nonlinear Newton linesearch algorithm needs to converge. Further investigation into why this is the case is warranted.

In one of the investigated scenarios adipose tissue is modeled using a volumetric mesh and the Robin boundary conditions are applied on its outside surface. We conclude that this approach leads to similar results as a partitioning of the epicardial surface into two regions with different penalty parameters and therefore a volumetric representation of the adipose tissue is neither necessary nor practical. Based on our results, the sliding contact formulation appears to be advantageous in both computational cost and accuracy.

Modeling and Simulation of Pharmaco-Mechanical FSI for an Enhanced Treatment of Cardiovascular Diseases - Part I: Modeling Aspects

Nurani Ramesh, Sharan; Uhlmann, Klemens; Balzani, Daniel 14:20
Ruhr University Bochum

Diseases of the vasculature are routinely treated using antihypertensive drugs in clinical setups. However, certain combinations of drugs have been found to have undesirable effects [1]. Numerical simulations of the mechanical response of healthy and pathogenic arteries affected by drugs are important in-silico tools to better understand the mechanical behavior of atherosclerotic arteries under the influence of antihypertensive agents. This entails an accurate description of the absorption and diffusion of drugs in the arterial walls in conjunction with a suitable material model. Accordingly, a coupled pharmaco-mechanical model, which extends the smooth muscle cell (SMC) model by Uhlmann and Balzani [2] by including a reaction-diffusion model for the transmural drug transport, is developed. In particular, the effects of calcium channel blockers on SMC contraction are incorporated by defining the drug-altered intracellular free calcium concentration and the calcium-dependent activity of the enzyme Mysoin Light Chain Kinase(MLCK). Residual stresses are accounted for using models for stress-driven anisotropic growth and arterial wall remodeling [3]. Algorithms for the implementation in finite element programs will be presented. Simulation results of atherosclerotic arteries under intravascular pressure will be discussed with regard to the potentially negative influence of antihypertensive drugs on atherosclerotic plaques.

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Modeling and Simulation of Pharmaco-Mechanical FSI for an Enhanced Treatment of Cardiovascular Diseases - Part II: Numerical Methods, Software, and Results

Saßmannshausen, Lea (1); Klawonn, Axel (1,2); Knepper, Jascha (1,2); Heinlein, Alexander (2) 14:40
1: University of Cologne
2: TU Delft

Today, cardiovascular diseases are among the leading causes of death worldwide. With a special focus on the treatment of hypertension and the clinical consequences thereof, the computational modeling of fluid-structure interaction with pharmaco-mechanical effects becomes increasingly relevant. A fluid-structure interaction (FSI) model is extended to reflect the influence of drugs on the structural properties of, possibly atherosclerotic,arterial walls. More precisely, a coupled pharmaco-mechanical model which extends the smooth muscle model of Uhlmann and Balzani (2023) by including a reaction-diffusion model for the drug interaction, is incorporated in the FSI model, leading to a fully coupled fluid-structure-chemical interaction model, denoted as FSCI. Furthermore, the FaCSI factorization (introduced by Deparis, Forti, Grandperrin, and Quarteroni in 2016) for a fluid-structure interaction problem is modified to include the pharmaco-mechanical coupling. The resulting linearized FSCI system is then solved with a Krylov method where the arising block subsystems of the fluid, the geometry and the structure-chemical interaction are preconditioned by two-level overlapping Schwarz precondtioners with GDSW-type (Generalized Dryja–Smith–Widlund) coarse spaces. These highly-scalable parallel GDSW (Generalized Dryja–Smith–Widlund) coarse spaces have been implemented in the solver framework FROSch (Fast and Robust Overlapping Schwarz), developed at the University of Cologne, TU Delft, and TU Freiberg; FROSch is part of the software library Trilinos. In this talk, results of FSCI for a realistic setting are investigated using a finite element implementation based on our software FEDDLib (Finite Element and Domain Decomposition Library) and Schwarz preconditioners from the Trilinos package FROSch.

SimLivA - A Data-Integrated, Continuum-Biomechanical Framework for In-Silico Staging of Ischemia-Reperfusion Injury During Liver Transplantation

Mandl, Luis (1); Gerhäusser, Steffen (1); Lambers, Lena (1); Dahmen, Uta (2); König, Matthias (3); Tautenhahn, Hans-Michael (4); Ricken, Tim (1)

1: University of Stuttgart
2: University Hospital Jena, Friedrich Schiller University
3: Humboldt-Universität zu Berlin
4: University Hospital Leipzig

15:00

Liver transplantation is the only therapy to treat acute and chronic end-stage liver diseases, but challenges arise with an increasing number of elderly and multi-morbid donors and recipients. Grafts from such donors frequently exhibit compromised quality due to hepatic steatosis, affecting tissue structure, perfusion, metabolism, and overall organ function. Marginal grafts, characterized by hepatic steatosis, present a dilemma for surgeons who must decide whether to accept or reject the organ, increasing either the recipient's postoperative risk or the risk of mortality on the waiting list. Two major challenges for these marginal liver grafts are the storage between organ procurement and transplantation (cold ischemia) and the damage during reperfusion, known as ischemia-reperfusion injury (IRI).

Computational continuum-biomechanical modeling of tissue represents an emerging approach to resolve the intricate interplay of deformation, perfusion, and function in the liver (cf.[1]). The liver lobules as the functional liver units are expressed as a homogenized porous medium based on the theory of porous media (TPM; cf.[2]). Together with the cellular metabolic processes, a poroelastic multiphase and multiscale function-perfusion model is obtained (cf.[3, 4]), coupling partial differential equations on the lobular scale with ordinary differential equations on the cellular scale. Blood is given as a fluid phase with anisotropic perfusion, whereas healthy liver, necrotic, and fatty tissue are regarded as solid phases. The energy balance, cell death, and cellular functionality of each hepatocyte can be modeled via systems biology approaches. This yields a spatiotemporal model which may be used to describe the damage caused by oxygen and nutrient depletion during ischemia.

The efficacy of this approach stems from the integration of both experimental and clinical data for parameterization and validation, combined with prior knowledge in the computational models. This significantly enhances its real-world applicability for the assessment of IRI based on the simulation of the spatiotemporal evolution of the considered phases and solutes. Image analysis, both classical and machine-learning-based, extracts liver lobule geometry and steatosis zonation patterns from histopathological images. Laboratory data provides initial and boundary values, alongside information on the transplantation process, such as cold ischemia time. This framework offers predictive and patient-specific assessment of IRI, thus representing a significant step towards a support tool for clinical decision-making (cf.[1]).

[1] Christ et al. Frontiers in Physiology 12:733868(2021)

[2] Ehlers:„Foundations of multiphasic and porous materials" in Porous Media: Theory, Experiments and Numerical Applications(2002).

[3] Ricken et al. BMMB 14:515-536(2015)

[4] Lambers et al. BMMB, accepted for publication(2023)

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

Organizer(s): Eberhard, Peter *(Universität Stuttgart)*

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

Date: March 19, 2024 14:00–16:00
Room: G26/H1
Chair(s): Eberhard, Peter
Bestle, Dieter

Learning bifurcation structures in the small-data limit using reservoir computing

Yadav, Manish; Stender, Merten 14:00
TU Berlin

Mechanical systems are known to exhibit complex dynamical behavior and may undergo qualitative changes to their dynamics under parameter changes. Mapping out complete bifurcation diagrams either numerically or experimentally is resource-consuming, or even infeasible. Taking a data-driven approach, this study investigates how bifurcations can be learned from a few system response measurements. Particularly, the concept of reservoir computing (RC) is employed. As proof of concept, a minimal training dataset under the resource constraint problem of a Duffing oscillator with two different external forcings has been provided as training data. Our results indicate that the RC not only learned to represent the system dynamics for the trained external forcing, but it also manages to provide qualitatively accurate and robust system response predictions for completely unknown parameter regimes outside the training data.

Hybrid Modelling of Multibody Systems: Application of Two Discrepancy Models for Trajectory Prediction

Wohlleben, Meike (1); Muth, Lars (1); Sextro, Walter (1); Eberhard, Peter (2) 14:20
1: Paderborn University
2: University of Stuttgart

A precise physical model relies on a correct representation of relevant phenomena and can be easily adapted to changing system parameters once set up. In contrast, with data-driven models, physical phenomena do not need to be explicitly modelled, because the models automatically capture relevant effects through measurements. However, many measurements under the considered operating conditions are required to sufficiently represent the possible parameter space.

By combining these modelling methods, hybrid models can be created, in which it is possible to influence which disadvantages and advantages of the respective modelling method are retained, and which are balanced out. One example for hybrid models are discrepancy models. These contain a physical model of the basic system behaviour. Inaccuracies due to unmodelled phenomena, parameter inaccuracies or numerical errors are then compensated using a data-driven model.

For the modelling of a multibody system, two methods of discrepancy modelling are applied in this work. The first method is based on the discrepancy of the state vector. The second method is based on the discrepancy of the time derivative.

An excited four-bar linkage with friction in the joints serves as an application example. Measurements of both displacement and acceleration are taken at the coupler point of the four-bar linkage. Subsequently, the two presented methods are applied, and the results are compared with respect to accuracy and calculation time. Furthermore, the preconditions for the application of the respective method are discussed.

Artificial Recurrent Model for Parameter Identification of Dynamic Systems

Bielitz, Timo; Bestle, Dieter
BTU Cottbus-Senftenberg

14:40

The identification of parameter values generating a specific solution is one of the fundamental tasks in dynamic system analysis. Therefor, classically either a corresponding mathematical model is formulated based on physical principles or a real-world experiment may be set up. The identification is then an iterative process of changing parameter values $\boldsymbol{p}$ and comparing the resulting system behavior $\boldsymbol{x}(t)$ with a desired one until both coincide. However, if the expense of this procedure increases caused by high system complexity or if the system dynamics is even unknown, more sophisticated approaches have to be taken [1] or machine learning strategies [2] may be applied.

Here, a machine learning approach will be taken which also reflects dynamic properties. Especially, in a nonlinear dynamic system the solution is given by the phase flow $\boldsymbol{x}(t)=\varphi(t;\boldsymbol{x}_0,\boldsymbol{p})$, which maps a state $\boldsymbol{x}_0$ onto all consecutive ones $\boldsymbol{x}(t)$. However, if the system equations are unknown, the phase flow is unknown as well. This is why the use of a neural network with recurrent cells involving adjustable weights is proposed. The recurrence of this network is then able to account for the causality of the phase flow. To perform a fully equivalent mapping, the weights of the model are iteratively trained with the aim to minimize the loss reflecting the difference between some training trajectories and the corresponding network output calculated autoregressively from the same initial conditions.

Once the recurrent model is trained, the identification task may be executed for a particular solution trajectory where the goal is to find the corresponding parameter values. Therefor, two different approaches are proposed and compared: On one side, an evolutionary optimization algorithm starts from randomly guessed candidates of parameter values and updates them iteratively based on their corresponding reconstruction loss. On the other side, the identification is performed by the network itself. Two additional weights, which have been ignored so far and represent the parameter values, are now trained with the aim to rebuild the desired solution trajectory while keeping all other, already trained weights of the network unchanged. Both suggested schemes have been applied to identify the length of a nonlinear mathematical pendulum and the preload of a translational return spring attached to it.

[1] Vega, D. C., Paz, S. R., Ornelas-Tellez, F. & Rico-Melgoza, F. J. (2018). System Parameters' Identification and Optimal Tracking Control for Nonlinear Systems. *IFAC-PapersOnLine*, 51, 431-436.

[2] Rudi, J., Bessac J. & Lenzi A. (2021). *Parameter Estimation with Dense and Convolutional Neural Networks Applied to the FitzHugh-Nagumo ODE*. arXiv:2012.06691.

A deep learning approach to calculate elementary effects of Morris sensitivity analysis

Raj, Rohit; Tismer, Alexander; Gaisser, Lukas; Riedelbauch, Stefan
University of Stuttgart

15:00

Shape optimization of a multi-component hydraulic turbomachinery is cumbersome and computationally expensive due to the number of computational fluid dynamics (CFD) simulations required. Sensitivity analysis (SA) is crucial in reducing the model parameters. Morris sensitivity analysis (1) is used to screen the essential parameters, requiring only a few points to identify the most important input parameters from many parameter sets. It offers cheaper computations needed to perform SA. This method is based on the so-called elementary effects (EE), which calculates the derivatives using the finite difference method. The drawback of this method is that in case of a failed simulation, the whole trajectory consisting of n+1 simulation results needs to be thrown away instead of just the failed simulation result.

In this work, an alternate way to calculate the Morris method's elementary effect (EE) has been tried using Deep Learning's (DL) backpropagation (2). To accomplish this, a supervised learning technique is implemented to map from inputs to outputs. The chain rule of differentiation is utilized to obtain the partial derivatives of the functions calculated by the trained DL model. As mentioned earlier, this approach solves the drawback, as it is not trajectory-dependent. The study concludes with an

observation that a model trained with fewer Morris samples cannot compute similar EEs as computed through finite difference approaches. On the other hand, a model trained with many training samples shows a promising result.

References

1. Morris MD. Factorial Sampling Plans for Preliminary Computational Experiments. Technometrics. 1991 May 1;33(2):161–74.

2. LeCun Y, Bengio Y, Hinton G. Deep learning. Nature. 2015 May;521(7553):436–44.

An iterative-closest-point algorithm for marker-free 3D shape reconstruction of tube-like continuum robots

Hoffmann, Matthias Klaus (1); Ding, Zhaoheng (2); Mühlenhoff, Julian (2); Sattel, Thomas (2); Flaßkamp, Kathrin (1)

1: Saarland University
2: TU Ilmenau

15:20

Continuum robots, like those constructed from curved concentric tubes, have emerged as a promising technology in the medical field due to their potential for intricate procedures such as medication delivery and biopsies. The mechanisms of these robots show potential for precise navigation around challenging anatomical structures like vessels. Despite the availability of first-principle models, accurately predicting the final shape of such continuum robots remains a challenge, primarily since critical effects such as concentricity deviation, hysteresis, or non-linear material behavior are neglected in the modeling process. Furthermore, assessing the error between the predicted and actual robot shape is a challenging task, as accurate measurements of the robot are mandatory. Automated photogrammetry-based measurements in multiple images, for example, based on the detection of interest points, are difficult to realize, necessitating the manual identification of corresponding points to reconstruct the robot's three-dimensional structure. This contribution introduces an iterative-closest-point algorithm, leveraging optimization techniques to align a 3D curve as the reconstruction with images of the robot. The algorithm facilitates arbitrarily fine and equidistant sampling of the robot, addressing and overcoming limitations of widely used reconstruction techniques.

Optimization of Crash Box Design in Crashworthiness Analysis Using Reinforcement Learning

Borse, Aditya; Gulakala, Rutwik; Stoffel, Marcus

RWTH Aachen University

15:40

This study focuses on the optimisation process of crash box design. The design optimisation process is resource-intensive and requires multiple dynamic simulations. Numerous design parameters can be varied to satisfy the crashworthiness objectives [1]. Therefore an intelligent and robust ML framework has been developed. This framework can be employed to assist in the optimisation of various crashworthiness components with different crashworthiness objectives.

Here, a reinforcement learning-based (RL) machine learning framework is developed. It consists of a FEM surrogate and reinforcement learning (RL) environment. The FEM surrogate is trained using data from FEM simulations as well as synthetic data generated by a Generative Adversarial Network (GAN) [2]. An inverse problem is solved for optimising the geometrical parameters of the boundary value problem while the RL is receiving input from the FEM surrogate. RL has proven to be accurate in many fields due to its ability to explore and exploit the learned dynamics. Conventional algorithms require numerous iterations and tuned functions to achieve appropriate results and need to be initialised after a slight change in the problem [3]. Due to an optimisation of input parameters in an inverse problem, RL is chosen for the present investigation.

For the simulation data needed, the crash box is designed with linear first-order accurate four nodal shell elements, which are suitable for large deformations and arbitrary large rotations and based on the Mindlin Plate theory [4]. Also, bilinear elastoplastic material along with geometrical nonlinearity is used to simulate the dynamic deformation process.

The RL agents learn to vary the crash box design parameters and search for the optimal parameters. The optimal parameters are based on the user-defined crashworthiness objectives.

SPP 2410: Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness

Organizer(s): Rohde, Christian *(University of Stuttgart)*

DFG-PP 2410: Hyperbolic Balance Laws in Fluid Mechanics: Complexity, Scales, Randomness

Date: March 19, 2024 14:00–16:00
Room: G16/215
Chair(s): Rohde, Christian

Convex integration applied to the compressible Euler equations: non-uniqueness and admissibility criteria

Markfelder, Simon 14:00
JMU Würzburg

In the past years, results based on a technique called convex integration have drawn lots of interest within the community of mathematical fluid mechanics. This technique allows to prove existence of infinitely many solutions for the multi-dimensional compressible Euler equations. All these solutions satisfy the energy inequality which is commonly used in the literature to identify physically relevant solutions. On the other hand, intuitively at least some of the infinitely many solutions still seem to be non-physical. For this reason one has studied additional admissibility criteria regarding maximal energy dissipation, to no avail: such criteria do not select the solution which is expected to be the physical one.
In this talk we give an overview on the aformentioned non-uniqueness results and we explain why maximal dissipation fails to single out the solution which is presumably the physical solution.

On Non-Strict Hyperbolic Systems and Related Wave Phenomena

Thein, Ferdinand 14:30
RWTH Aachen University

The theory of hyperbolic PDEs in one space dimension focuses to a large extent on strict hyperbolic system.
The key property of such systems is that there are distinct and ordered eigenvalues which do not change their ordering across waves. However, in a recent work a symmetric hyperbolic system modeling two phase flow was investigated. This model is non-strictly hyperbolic in the sense that eigenvalues may coincide and change their ordering across waves. This property leads to complicated wave phenomena barely studied in the literature. In this talk we want to revisit this system and its complex properties. Furthermore we suggest a simpler generic model which exhibits similar features. Thus it is demonstrated that these phenomena are not only related to two phase flows but may be a general feature of non-strict hyperbolic problems.

Asymptotic Preserving Numerical Methods for Linear Kinetic Transport Equations Based on Upwind SBP Schemes Combined with Multiderivative RK Methods

Ortleb, Sigrun 15:00
University of Kassel

Kinetic models describe a wide range of physical processes relevant to natural and engineering sciences where a large number of particles is involved. Compared to macroscopic models describing the behavior of averaged quantities in terms of densities, kinetic models are closer to particle descriptions by operating on an intermediate level between the particle perspective and the macroscopic behavior. More detail to specific phenomena and a more accurate mathematical description of the problem may thus be provided by kinetic models for a broad range of phenomena in the areas of rarefied gases, radiative transfer and turbulence modelling. Kinetic models possess a multiscale nature with respect to the Knudsen number, i.e. the ratio of the mean free path of particles and the characteristic length. As this multiscale nature may vary locally in space and time, a long-standing multiscale approach is

given by asymptotic preserving schemes passing from the kinetic to the macroscopic model on the discrete level. Hereby, a specific technique for the construction of asymptotic preserving schemes is micro-macro decomposition. Recently, efficiency of numerical schemes for specific kinetic models modeling radiative transfer has been increased by a Schur complement strategy by Peng and Li [Siam J. Sci. Comput. 2021] allowing to implicitly discretize those terms in the micro-macro equation which are linked to diffusion in the asymptotic limit. This work rigorously proves unconditional stability for low order schemes with additional numerical verification for higher order approximations, meaning that for small scaling parameters near the macroscopic limit arbitrarily large time steps may be chosen. Upwind Summation-by-Parts (SBP) schemes provide a generic framework to construct robust, structure preserving approximations of higher order. For upwind SBP space discrtizations in combination with implicit-explict Runge-Kutta (RK) time integrators, it is possible to rigourously extend the theoretical unconditional stability result by Peng and Li to higher order spatial discretizations using the energy method. Multiderivative RK methods include higher order derivatives within their stages, similar to a Taylor series method. This allows for higher order methods with fewer stages as well as for the construction of unconditionally strong stability preserving high order schemes. Under specific conditions on the multiderivative RK scheme, unconditional stability for linear kinetic transport may be achieved as well. In this talk, we thus discuss the combination of upwind SBP space discretization and implicit-explicit multiderivative Runge-Kutta time integrators for linear kinetic transport equations.

Convergence of FE schemes for compressible flows via dissipative weak solutions

Öffner, Philipp
Clausthal University of Technology

15:30

Many problems in computational fluid dynamics are described via the compressible Euler or Navier-Stokes (NS) equations.
Recently, dissipative weak (DW) solutions have been introduced as a generalization to classical solution concepts. In a series of works, DW have been established as a meaningful concept from the analytical and numerical point of view. DW solutions do not have to fulfil the equations weakly but up to some defect and oscillation measures. They are a natural extension of classical solutions since DW solutions coincide with them if either the classical solution exists, referred to as the weak-strong uniqueness principle, or if they enjoy a certain smoothness. Further, they can be identified as limits of consistent and stable approximations and convergence towards DW solutions have been demonstrated for several structure-preserving numerical methods in the context of the Euler and Navier-Stokes equations.

In this talk, we give an introduction to the concept of DW solutions and summarize recent results inside this framework. We consider, in particular, high-order FE schemes and demonstrate convergence to DW solutions for the multi-dimensional Euler equations. To this end, it is crucial that structure-preserving properties, such as positivity preservation and entropy inequality hold, and the schemes are consistent with the underlying PDE. We show how to ensure them and in numerical simulations, we verify our theoretical findings. Importantly, the applicability of DW solutions extends beyond the Euler and Navier-Stokes equations. As we conclude, we offer a glimpse into the future, discussing potential developments in this evolving field.

Contributed Sessions

S01: Multi-body systems, mechatronics and robotics

Organizer(s): Oveisi, Atta *(Ruhr-Universität Bochum)*
Nestorovic, Tamara *(Ruhr-Universität Bochum)*

S01.01: in Focus SPP 2353: Daring More Intelligence – Design Assistants in Mechanics and Dynamics

Date: March 20, 2024 16:30–18:30
Room: G22/217
Chair(s): Eberhard, Peter

Characterization of the behavior of slender, soft robots

Schindler, Leon; de Payrebrune, Kristin M.; Seis, Robin 16:30
RPTU Kaiserslautern-Landau

In recent years, soft robotics has developed into an innovative and increasingly important area within robotics. The basic idea in this novel field is to use soft materials. These materials have a softness comparable to human tissue. With these materials, soft robots are capable of adapting to and interacting with their environment without extensive use of sensor systems. Their field of application therefore ranges from safe human-machine interaction to medical aids, for example as a surgery tool. For practical applications, it is important to understand and determine the deformation of a soft robot as a function of various input parameters. A universally applicable and pneumatically actuated bending actuator was used as a real example. It was designed at the Institute of Computational Physics in Engineering (CPE) at the RPTU Kaiserslautern-Landau. In the case of this bending actuator, the input parameters include, for example, the set air pressure in the actuator and its material stiffness. The deformation behavior can be determined using two approaches. On the one hand, experiments can be carried out. On the other hand, it is possible to set up and run simulations. Both options were used.

The simulations conducted simplify the investigation of the deformation behavior in such a way that the influence of different parameter variations can be carried out efficiently and in a time-saving manner. One disadvantage is the model of the bending actuator used. The model is not capable of fully representing the complexity of a real bending actuator. For example, non-linear behaviors were simplified and approximated by linear submodels. However, experiments show the actual behavior of the bending actuator with its non-linear characteristics.

With the help of simulations, it is possible to investigate the deformation behavior as a function of various input parameters. In addition, the impact of individual parameters on the deformation can be highlighted. The comparison between experiment and simulation reveals errors. In a further step, these can be understood and corrected.

Real-time Models for Systems with Costly or Unknown Dynamics

Bestle, Dieter; Bielitz, Timo
BTU Cottbus-Senftenberg

16:50

Many applications like model predictive control, observers, gaming, visualization of systems with human interaction or driving simulators require real-time simulation where the computer model can be executed at least as fast as the underlying physical system. However, as the complexity of models grows, e.g. in case of flexible multibody dynamics accounting for body elasticity, this becomes harder even with high-end computers and parallel computing. Also the modeling itself may become too cumbersome to come up with causal models, especially in industrial applications, or modeling may even be impossible due to unknown physical effects. In such cases, data-based modeling with AI-strategies may be an alternative to come up with real-time capable simulation models.

The idea is rather simple: Starting from randomly chosen initial conditions and system parameters $\mathbf{p}$, we may first generate data $\mathbf{x}_i=\mathbf{x}(t_i)$, $\mathbf{u}_i=\mathbf{u}(t_i)$, i=0,1,2,…, offline for state $\mathbf{x}(t)$ and control $\mathbf{u}(t)$, either by costly simulations of a given causal model or measured from a physical experiment. Based on these trajectory data, we may then generate approximations for the state function of differential equation $d\mathbf{x}/dt=\mathbf{f}(\mathbf{x},\mathbf{u};\mathbf{p})$ by 1st order finite differences $\mathbf{f}_i(\mathbf{x}_{i+1}-\mathbf{x}_i)/(t_{i+1}-t_i)$ or any higher-order differences. These samples $(\mathbf{x}_i,\mathbf{u}_i,\mathbf{p}),\mathbf{f}_i$ serve then as training and test sets to find an AI-model $\mathbf{f}_{AI}(\mathbf{x},\mathbf{u};\mathbf{p})$ as substitute for the original or unknown state function. Due to the short execution time of AI-models like artificial neural networks (ANN) or random decision trees, the approximate state equation $d\mathbf{x}/dt\mathbf{f}_{AI}(\mathbf{x},\mathbf{u};\mathbf{p})$ can finally be solved faster than real time. At least for short time horizons as required in controlled systems or systems with feedback, the prediction quality of the learned model is sufficient and overcomes the bottleneck of limited system complexity.

A first test of the proposed method with ANN applied to the Duffing equation has shown high conformity of predicted and directly simulated trajectories, both integrated with the Dormand-Prince scheme *ode45*. The same holds for a second test case, the multibody system model of a closed-loop mechanism called lambda-robot. The promising results motivate the study of more complex multibody systems where real-time capability becomes an issue.

Multi-Criteria Hydraulic Turbine Optimization using a Genetic Algorithm and Trust-Region Postprocessing

Rentschler, Tobias (1); Berkemeier, Manuel Bastian (2); Tismer, Alexander (1); Peitz, Sebastian (2); Fraas, Stefan (1); Riedelbauch, Stefan (2); Sextro, Walter (2)
1: University of Stuttgart
2: Paderborn University

17:10

This study investigates the application of CoMPrOMISE, a derivative-free trust-region optimizer, to the complex optimization of hydraulic turbines with multiple, possibly conflicting, objective functions. As is usual in multi-criteria optimization, the goal is the identification of optimal trade-offs between those objectives, constituting the so-called Pareto set.

Traditional optimization methods often require a large number of function evaluations, which can be prohibitively expensive for hydraulic turbines, where each evaluation involves a time-consuming fluid simulation. For the same reason, gradient-based methods cannot be directly applied.

CoMProMISE is a trust-region solver that utilizes local surrogate models to approximate gradient information with a minimal number of function evaluations. This technique has demonstrated efficiency on simple test problems. Our contribution now aims to evaluate the performance of CoMProMISE and the well-established Genetic Algorithm NSGA-II on a more challenging, highdimensional application.

The case study uses a detailed model of an axial turbine characterized by thirty design parameters that cover multiple aspects of the turbine's design and functionality. The flow within the turbine is simulated using OpenFOAM, a powerful open source computational fluid dynamics tool. The NSGA-II algorithm is applied to optimize two main objectives: increasing the efficiency of the turbine and minimizing the cavitation volume, which is essential for the performance and durability of the turbine.

Additionally, there are constraints associated with the design head which have to be fulfilled. It provides an initial approximation of the Pareto set, where efficiency and cavitation reduction should be balanced in such a way that neither criterion can be improved upon without detrimentally affecting the other. However, as a heuristic algorithm, NSGA-II requires a large amount of function evaluations and there is no formal convergence guarantee. We hence use points from the approximate Pareto set to initialize CoMPrOMISE for further investigation. This combined method evaluates whether the NSGA-II algorithm has reached full convergence. If convergence is not achieved, it provides alternative solutions that are closer to the true Pareto set.

The primary objective of this investigation is to assess the real-world applicability of CoMPrOMISE and the synergy potential of different optimization techniques in the design process of a hydraulic turbine. To investigate whether an integrated optimization strategy can yield more efficient and effective turbine designs, CoMPrOMISE is applied to either improve or verify solutions from the Genetic Algorithm.

Exploring the Optimal Leg-Stiffness in a 2D Monoped

Raff, Maximilian; Remy, C. David
University of Stuttgart

17:30

In the fields of robotics and biomechanics, the integration of elastic potentials such as springs and tendons in legged systems has long been recognized for its role in fostering energy-efficient locomotion. Yet, a persistent challenge remains: designing a robotic leg that reliably performs well across diverse operating conditions, especially varying average forward speeds. It is not even clear whether, for such a range of operating conditions, the stiffness of the elastic elements needs to be varied or if a similar performance can be obtained by changing the motion and actuation while keeping the stiffness fixed.

The goal of our investigation is to conduct an extensive parametric study on a monopedal robot that is featuring a linear leg-spring (stiffness k) operating in parallel to the leg's actuator (parallel elastic actuation).
Our primary focus is to identify the influence of the parameter k on the energy efficiency of the robot while performing a periodic hopping motion (gait). This is done within an optimal control framework, which generates motions and actuator inputs that minimize the energetic cost of transport. We construct this periodic trajectory optimization problem by discretizing the actuation space with B-splines and solving a multiple shooting problem. The optimization problem is parameterized by k and the desired average forward speed v.

In this contribution, we present a framework to efficiently navigate the extensive optimization landscape for various parameters and generate a surface illustrating optimal gaits. This framework relies heavily on numerical continuation methods. These techniques offer computationally efficient analyses, aiding in visualization and insightful analysis of the surface. The ultimate goal is to contribute valuable insights that facilitate the efficient design of robotic legs adaptable to diverse locomotive demands.

Simulation of Thermical and Dynamical Behavior of High-Precision Optical Systems

Eberhard, Peter; Kurcics, Mark
University of Stuttgart

17:50

For the predictive simulation and optimization of high-precision optical systems a complex multidisciplinary simulation needs to be set up which considers besides the optical behavior also the dynamical and thermical behavior. There exist many couplings, e.g. when thermal energy is floating through the system, deformations due to thermal stresses occur which in turn change the geometry and the optical path. However, not only the optical ray tracing is involved by heat but also the optical properties of the material of lenses are changed. Care in all details needs to be spent, e.g., the heat may not be just included point-wise on the lenses and mirrors but a precise modelling of the laser-rays must be investigated and introduced. In this talk an overview of an framework is presented which can efficiently and precisely simulate such effects. For a system with several lenses, the distortions of

optical images based on dynamical thermal loads are shown. Such a framework allows not only simulations but can also be extended to perform optimizations, uncertainty analyses or it can be coupled to control algorithms or model order reduction.

S01.02: Robotic Applications

Date: March 21, 2024 08:30–10:30
Room: G22/217
Chair(s): Oveisi, Atta
Pal, Amit Kumar
Nestorovic, Tamara

Multimodal 3D Reconstruction of Icy Surfaces for Robotic Applications: A Dataset and Analysis

Kaastrup-Hansen, Amalie (1); Pham, Huy Xuan (1); Kayacan, Erdal (2) 08:30
1: Aarhus University
2: Paderborn University

Three-dimensional (3D) reconstruction stands as a cornerstone in diverse robotic applications, serving critical roles in scene understanding and navigation. Typically, LiDAR has been a key player in generating precise point clouds of the environment, supplying essential data for these applications. Nevertheless, the efficacy of LiDAR sensors is notably hampered in challenging conditions, for example, the presence of water or icy surfaces. The intricate interplay between laser beams and icy or non-ideal surfaces can lead to signal degradation, distortion, or even complete signal loss, adversely impacting the accuracy and reliability of the 3D reconstruction process. The reflective and refractive properties of ice, coupled with its variable surface conditions, introduce complexities that traditional LiDAR sensors struggle to navigate.

This paper investigates the limitations of LiDAR in detecting and reconstructing an icy surface, and proposes a multimodal approach for improved 3D reconstruction using different sensors. To complement the LiDAR, we aim to identify the regions with presence of ice on the surface where LiDAR is expected to perform less accurately, and compensate by leveraging visual and depth cameras for improved understanding of the surface texture, and adding a thermal camera to provide valuable temperature information. We explore the integration of diverse data sources to enhance the robustness of reconstruction algorithms in challenging environments. Our study investigates how the fusion of data from different sensors can effectively capture the intricate details of icy surfaces, ensuring a more accurate understanding of the environment.

The experimental results aim to benchmark the accuracy of detection and 3D reconstruction methods for icy surfaces using different sensor modalities. We discuss the insights gained from our study and highlight the potential impact on various robotic tasks, emphasizing the importance of robust 3D reconstruction in adverse environmental conditions. To facilitate further research in this domain, we also contribute an open-source dataset comprising synchronized recording of multiple sensors (LiDAR, RGB camera, depth camera, thermal camera) on diverse icy surfaces and objects.

In conclusion, this paper presents an effort in addressing the challenges of 3D reconstruction of icy surfaces by leveraging multiple sensor modalities, thereby contributing to the development of more resilient robotic systems capable of navigating and understanding environments with icy conditions.

Imitation learning for graph search algorithms and super-smooth spline in navigation of mobile robots: a case study on Turtlebot

Oveisi, Atta; Nath, Aswin; Sülecik, Bilgehan; Pal, Amit Kumar; Nestorović, Tamara 08:50
Ruhr University Bochum

In the realm of robotics, the era of autonomous driving is marked by unparalleled innovation and exploration. The first segment of this study delves into techniques for robot navigation, with a particular focus on the pivotal role played by the Robot Operating System (ROS) in facilitating seamless

communication and coordination among various faculties of a mobile robot. Planning algorithms constitute an integral aspect of robot navigation, and this work initially explores and compares different classical planning algorithms, including the A* algorithm. The widely studied mobile robot, Turtlebot3, is employed to test the capabilities of these algorithms, empowered by cutting-edge sensors and ROS to navigate intricate environments with precision and adaptability guided by various planning algorithms. Many planning algorithms generate trajectories with sharp turns, e.g. graph search methods on coarse maps leading to challenges such as increased time consumption in actuation and jerky movements due to physical limitations on the turning speed of the mobile robot. Path smoothing, investigated in this work, is employed to mitigate these issues. The challenges and advantages of using spline interpolation for path smoothing are also explored. The second part of this study capitalizes on the benefits of imitation learning in navigation. Traditional planning and smoothing algorithms are computationally intensive. Instead of executing these algorithms directly on the embedded hardware of the robot, which often has limited computational capacity, they are implemented in a simulated environment using a model of the mobile robot across various scenarios. The robot's behavior is simulated in different environments with multiple obstacles and goal locations, allowing classical planning algorithms to learn optimal paths. From the simulation data, a supervised learning problem is formulated and solved using an artificial neural network. The trained network is then deployed on the real robot system. To validate this approach, the performance of the actual classical planner and that of the trained neural network is compared in real-time. This technique holds the potential to leverage simulation-based training and neural networks to enhance navigation efficiency while respecting the hardware limitations of the robot, consequently saving energy for repetitive use.

Effectiveness of lightweight neural network in imitating model predictive controllers in robotics

Pal, Amit Kumar; Oveisi, Atta; Nestorović, Tamara 09:10
Ruhr University Bochum

The success of model predictive controllers (MPC) is well-known in the field of control and robotics to the extent that MPC has become an industry standard for different sectors, such as automated driving. The main advantage of using MPC is that the dynamics of the system can be taken into account to perform predictions over the state space manifold and use the predicted trajectory to construct an optimal problem that glides the system states toward a final state while different constraints can be integrated into the control system. This approach is proven to improve the safety and reliability of the controllers. However one of the major drawbacks is that MPCs are generally computationally more complex than traditional model-free approaches. This increases the requirement for capable hardware to implement the MPC online, which might be challenging for small mobile robots with limited power due to space and budget constraints. Motivated by the aforementioned challenges of realizing MPC in real-world applications, this paper explores the feasibility of training feedforward neural networks to imitate MPC controllers in simulation and then deploy the trained networks in the actual system with computationally affordable processors that comply with the limited power consumption. This methodology has massive potential to reduce the inference cost from the controller, especially when used repetitively for any specific task. This is because the computational complexity of the MPC is much more than the forward pass of a neural network. The cost-effectiveness of the proposed approach in this paper is proven numerically on a benchmark problem. Also, this method can be implemented by training the MPC controller on an actual system once and then training the network to imitate the MPC, which will further decrease the propagation of modelling bias.

Accordingly, in the rest of the paper, a systematic algorithm is presented that can replace the traditional MPCs for multiple inference after training. Several MPCs are implemented and the effectiveness of neural networks in imitating the MPCs is investigated. For the purpose of validation, the proposed imitation network performance is compared against costly MPC and the methodology is tested on an

actual inverted pendulum system. Moreover, potentially modern GPU-based hardware can be used to parallelize the forward pass for an even faster response from the controller.

S01.03: Dynamics and Multibody Systems – Fundamentals and Application

Date: March 21, 2024 14:00–16:00
Room: G22/217
Chair(s): Nestorovic, Tamara
Schmidtchen, Fabian

Optimisation of the hammer throw using parameterised synthetic motion kinematics in a multi-body system (MBS)

Schmidtchen, Fabian; Daniel, Christian; Tiedemann, Stefan; Woschke, Elmar 14:00
Otto von Guericke University Magdeburg

Hammer throwing is a motorically demanding sport in which the execution of the movement significantly influences the result, i.e. the throwing distance. There are many approaches for supporting technical training that are based on measurement technology and image capture. The accelerations and locus curves of the athlete and hammer are recorded and compared. In this article, these methods are supplemented by a MBS of the hammer throw. The kinematics of the hand movement is described using a parameterised synthetic trajectory. Scalar parameters in the approach allow the trajectory to be modified. With a MBS model of the wire cable and the hammer, the movement of the hammer can be determined by numerical time integration from the hand's trajectory. This results in the final throwing distance. Using heuristic methods, the parameters of the hand movement can be optimised for a maximum throwing distance. The optimised movement sequences can then be used to improve the athlete's training.

Development of a kinematic model for a free kinematic forming process to compute the tool trajectory

Ekanayaka, Virama; Hürkamp, André; Dröder, Klaus 14:20
TU Braunschweig

Certain restrictions in the linear forming process can be overcome through a free kinematic forming process, where the respective workpiece contour is formed by a tumbling or cyclic rolling movement of the forming tool. Due to this special kinematics, only a small part of the tool is ever in engagement with the workpiece, so the component is formed incrementally. The final geometry, therefore, does not have to be created in one stroke but can be carried out step by step in several partial strokes. In order to determine the optimal trajectory of the forming tool, the kinematic interplay between the workpiece, forming tool, and printing trajectory must be numerically captured in a mathematical model. The specific trajectory is based on the component being formed, as well as the actual geometry of the forming tool. In the subsequent control loop, the mathematical model is used to determine if the computed printing trajectory indeed produces the desired geometry of the workpiece. If the desired geometry cannot be achieved with the computed trajectory within a specified tolerance, the geometry of the forming tool has to be adjusted. This contribution details the approach to developing this kinematic model, which would then serve as an approximation to a detailed forming simulation, enabling a rapid assessment of the influence of the tool trajectory on the forming result based on the tool geometry.

Analysis of dynamic absorption system with a nonlinear damper described by a fractional-order model

Nešić, Nikola (1); Simonović, Julijana (2); Nestorović, Tamara (3) 14:40

1: University of Pristina, Serbia
2: University of Niš, Serbia
3: Ruhr University Bochum

Passive dynamic absorbers, also known as mass dampers, are typically investigated for their use in vibration suppression of buildings and other civil engineering structures. The proposed model consists of two rigid bodies, where the main body rests on a fractionally viscoelastic foundation. Additionally attached mass represents a nonlinear energy sink. The dynamical interaction and behavior of the two-degree-of-freedom mechanical system are described with a system of two coupled differential equations of the second order. The first equation contains the damping term described with fractional order derivative which has physical meaning for the range between 0 and 1. The second equation is nonlinear. The nonlinear fractional differential equation system is solved using incremental harmonic balance and the Newmark method, and results are compared. The influence of the resting foundation viscoelastic properties on the main body dynamics is analyzed. Additionally, the influence of the other system parameters variation, especially the mass/damper features, on amplitude-frequency response curves are analyzed and discussed.

Nonlinear dynamics of group rolling of bodies between concentric circle paths

(Stevanović) Hedrih, Katica 15:00

Mathematical Institute of Serbian Academy of Sciences and Arts

A group rolling, without sliding, of a finite number of heavy, homogeneous and isotropic balls or thin discs, of equal radius, between finite number of concentric circular paths of rolling and contacts is studied. The first circular path is stationary, and the others can rotate around a common axis, perpendicular to the common plane of the plane in which they lie. The configuration of this hybrid system is determined from independent generalized coordinates, with the number of independent generalized coordinates-central angles. The dynamic configuration of all bodies in rolling and contacts, without sliding is defined by central angles.

Expressions were determined for the instantaneous angular velocity of rolling, without slipping, of each of the subgroups of bodies rolling in a row, the relative angular velocity of rotation around their own axes, of each of the circular paths drawn by the rolling of the subgroups of bodies and along the first and subsequent circular paths, and in permanent contact with the next circular path.

The last in a series of circular path is rigidly connected to the shaft with which it rotates at the same angular velocity. While all the other circular trajectories, except for the last which is fixed, can easily rotate around the shaft, and their angular velocities are determined by kinetic connections with the rolling bodies.

The instantaneous rolling angular velocities of each of the subgroups of the body in rolling, without slipping, of the studied dynamics of the system were determined. A system of the number of nonlinear differential equations of the nonlinear dynamics of the system was determined, as well as the corresponding system of the number of equations of phase trajectories, and sketches of phase portraits and nonlinear dynamics were drawn. An analysis of the structure of singular points is given.

Based on the obtained results, a model of the construction of a multi-layer radial ball bearing was formed and the nonlinear dynamics of the rolling of subgroups of balls in the bearing was studied, as well as the interaction of the nonlinear dynamics of the rolling of the balls in the model of the radial

double-layer ball bearing and the nonlinear rotation of the shaft. The kinetic pressures on the - kinetic contact forces on the balls of the radial ball bearing were analyzed.

S01.04: Dynamic and Mechatronic Systems – Modelling, Simulation, Control

Date: March 21, 2024 17:40–18:40
Room: G22/217
Chair(s): Nestorovic, Tamara
Oveisi, Atta

Digital Twins of electrical switching devices for over-current protection with application to AI- assisted lifetime prognosis

Suresh Singhal, Dhruv (1); Boyaci, Aydin (2); Fidlin, Alexander (1) 17:40
1: Karlsruhe Institute of Technology
2: ABB AG, Germany

Energy transition and e-mobility require prognostics with advanced maintenance strategies for electrical switching and over-current protection devices. Digital Twins, which are virtual representations of physical entities, could be used for the purpose of health state prediction of electrical switching devices. In combination with data-driven lifetime models, digital twins could be used to implement AI-assisted prognosis systems for failure prediction. Circuit breakers are one of the key components of electrical switching devices used in electrical distribution networks. In spring-driven circuit breakers, switching is performed mechanically using an operation mechanism containing a complex kinematic chain. Simulation of switching operation requires multibody modeling of the underlying kinematic chain. The numerical complexity associated with multibody
models makes them difficult to implement as digital twins in circuit breakers. Even with state-of-the art technology, computational times for multibody simulations exceed those required for real-time operation of digital twins. In this study, we develop minimal models for an exemplary circuit breaker. We undertake measures to synchronize minimal models of the circuit breaker with the real system using sensor data for estimation of model parameters. Additionally, the minimal models are analyzed for their ability to reproduce system behavior with respect to aging effects such as changes in bearing/joint friction and clearances due to wear.

Visual Feedback Control for Positioning Support of a Rotary Crane

Kakuta, Yotaro (1); Paing, Min Set (1); Farrage, Abdallah (1,2); Kudara, Kazufumi (1,3); Takahashi, Hideki (3); Sasai, Shintaro (3); Sakurai, Hitoshi (3); Okubo, Masaki (3); Uchiyama, Naoki (1) 18:00
1: Toyohashi University of Technology, Japan
2: Assiut University, Egypt
3: Kobelco Construction Machinery Co., Ltd., Japan

A rotary crane moves a suspended load by vertical and horizontal boom motion, and has wide applications such as transportation tasks in construction sites and harbors. Operators are required to manually control them considering load-sway. Because of recent aging and severe decrease of skilled operators, automation of crane control is highly expected. Previous studies on crane control have investigated mainly motion planning and vibration suppression, and few studies have focused on operation support and vision-based control. Hence, this study considers a visual feedback control system for a rotary crane that employs a mounted camera to allow intuitive motion instructions for unskilled operators.

In the proposed system, the operator designates one position and its desired position by clicking them in the image captured by an onboard camera. Then, the system calculates the required boom horizontal and vertical motion by which the clicked one position to be at the desired position of the camera image. When this motion is conducted, load-sway typically occurs, and thus the load-sway reduction is required. Here, allowable load-sway is assigned first, and the system calculates the crane motion that keeps the load-sway less than the assigned magnitude by using a crane dynamic model.

The proposed system consists of a mounted camera and a control unit. The control unit includes an image processing unit and a controller. The mounted camera on the tip of the crane boom provides images of the ground and transmits them to the control unit. After clicking positions in the image, their pixel coordinate values are obtained. Then, the controller calculates the inverse kinematics of a crane by which required boom horizontal and vertical motions to move the designated position to the desired one.

The proposed system is implemented in an experimental environment to verify the effectiveness. The camera is mounted at the boom tip such that it always turns downward for obtaining an image of the ground without tilt. As a result, although the horizontal motion converges to the desired angle, the vertical motion exhibits an overshoot. In addition, the convergence time differs between horizontal and vertical motions. Hence, it is necessary to consider the above points in the controller design.

In conclusion, the effectiveness of the proposed system is confirmed experimentally. Further experiments will be conducted to see the load-sway magnitude which will be reduced by the estimation with a crane dynamics model.

A Spring-Mass Chain Multi-body Approach for Modeling Yarn Balloon Dynamics in Ring Spinning

Perez-Delgado, Yves Jesus; Beitelschmidt, Michael; Hossain, Mahmud; Abdkader, Anwar; Cherif, Chokri; Baloochi, Mostafa; Hühne, Ruben
TU Dresden

18:20

The ring spinning technology is widely used in textile industry to produce high-quality yarn. One of the challenges for higher productivity is the limited spindle speed due to friction in its conventional ring/traveler twisting system. However, it was shown recently that a superconducting magnetic bearing twisting system might overcome this limitation due to a significantly reduced friction, which allows the use of higher spindle speeds and thereby increase productivity.

To analyze the impact of speed increments on the yarn formation, it is crucial to model the yarn balloon dynamics. This is of particular importance as new challenges arise for such high-speed processes, including the increase in yarn tension due to higher centrifugal forces and an increased air resistance of the yarn itself.

Therefore, we developed a model based on a chain of springs and masses as an alternative to traditional continuous models. In the proposed model, each mass corresponds to a segment of the yarn, while the springs represent the interactions between adjacent segments. This discrete approach allows for a simplified simulation of the three-dimensional yarn balloon dynamics, leading to a reduced computational load, which allows to analyze the yarn path more easily under different conditions.

Acknowledgments:
This work was supported by the research program of the German Research Foundation, DFG (CH 174/61-1, BE 4791/5-1, and HU 1726/9-1) at the TU Dresden, Dresden, Germany.

S01.05: Modelling and Simulation of Dynamic Multibody Systems

Date: March 22, 2024 08:30–10:30
Room: G22/217
Chair(s): Pal, Amit Kumar
Oveisi, Atta

A non-stiff Lie group integrator for highly flexible structures with large rotations

Arnold, Martin; Tumiotto, Denise
Martin Luther University Halle-Wittenberg

08:30

Highly flexible slender structures may be described by geometrically exact beam models. With geometric integration methods structural properties of these beam models are kept on coarse space grids. Internal constraints refer to the neglection of shear effects and to inextensibility conditions.

The resulting model equations are non-stiff. They are formulated in a nonlinear configuration space to avoid singularities in the representation of large rotations. Classical non-stiff integrators for constrained systems may be adapted to this Lie group setting resulting in half-explicit Runge-Kutta Lie group integrators.

We construct methods up to order 5 and test them numerically for two classical benchmark problems from nonlinear beam theory. In the practical implementation, a 5th order method is equipped with step size control using an embedded method of order 4.

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A RATTLE integrator for the simulation of unilaterally constrained mechanical systems

Capobianco, Giuseppe (1); Breuling, Jonas (2); Leyendecker, Sigrid (1)

1: FAU Erlangen-Nürnberg
2: University of Stuttgart

08:50

The RATTLE integrator is a well-established method for simulating mechanical systems with bilateral constraints - multibody systems in particular. This talk presents an extension to the RATTLE integrator that can cope with unilateral constraints and even set-valued Coulomb friction. The proposed scheme can simulate impact-free motions, such as motions with persistent frictional contact, e.g. rolling motion, with second-order accuracy and prohibits numerical penetration of the unilateral constraints on position level. By that, it contributes to the development of higher-order integration schemes for simulating nonsmooth mechanical systems.

Case Study on Modeling Multibody Systems as Port-Hamiltonian Systems

Hochdahl, René; Drücker, Svenja; Seifried, Robert

Hamburg University of Technology

09:10

The trend for energy efficiency calls for smart solutions that connect mechanical, electrical and thermodynamic systems. For system development and analysis, a modeling method is necessary that can easily connect those different underlying domains into a unifying framework. The port-Hamiltonian framework promises to fulfill these requirements. It is a port-based modeling technique that breaks down a system into its core components and describes the energy flow between them. Therefore, it is inherently modular and connects multi-physics components via ports. As a result, a set of differential-algebraic equations is obtained which describes the system in redundant states.
Despite the progress in other fields of research, the port-Hamiltonian approach is so far not a very common approach in the multibody dynamics community. Therefore, this contribution gives a case study on modeling multibody systems as port-Hamiltonian systems. Our aim is to present prototypes of common building blocks of multibody systems, which can be connected to more complex mechanical systems. We consider systems with different properties, such as systems with and without kinematic loops. We compare the port-Hamiltonian modeling approach with conventional modeling techniques from analytical mechanics and discuss its advantages and disadvantages.
Due to the mentioned advantages of a simple connection of basic building blocks, we see further applications of the port-Hamiltonian approach in the multibody dynamics community, e.g. for control, model inversion and modeling flexible systems.

Structure-preserving time discretization of multibody systems with singular inertia matrix

Kinon, Philipp L.; Betsch, Peter

Karlsruhe Institute of Technology

09:30

Simulating the dynamics of a multibody system requires the choice of particular coordinates to parameterize translations and rotations. In doing so, the mathematical characteristics of the formulation are significantlyaffected, and the system's inertia matrix might become singular and/or configuration-dependent. Cases in whichthe inversion of the mass matrix is not admissible pose

difficulties to Hamiltonian formulations, which are the standard choice for the design of energy-momentum methods.

In this contribution we derive such a structure-preserving time integrator, inheriting energy- and momentum conservation in discrete time, based on a mixed variational principle. Livens principle (or sometimes called Hamilton-Pontryagin principle) unifies Lagrangian and Hamiltonian viewpoints on mechanics and features independent velocity and momentum quantities. In contrast to the canonical Hamiltonian equations of motion, the Euler-Lagrange equations pertaining to Livens principle circumvent the need to invert the mass matrix and to set up a Hamiltonian. These equations of motion are approximated by using (partitioned) midpoint discrete gradients, thus generating a new energy-momentum integration scheme for mechanical systems with singular and/or position-dependent mass matrix.

The derived method is second-order accurate, algorithmically preserves a generalized energy function and aims at the preservation of momentum maps corresponding to system symmetries. We apply the scheme to representative mechanical systems to validate the findings.

References:

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Vibration analyses of a mandible

Vulović, Aleksandra (1,2); Dimeski, Bojan (3); Geroski, Tijana (1,2); Saveljić, Igor (1,2); Nestorović, Tamara (3); Filipović, Nenad (1,2)

1: University of Kragujevac, Serbia
2: Bioengineering Research and Development Center (BioIRC), Serbia
3: Ruhr University Bochum

09:50

The main objective of this paper was to study the influence of vibrations on the human body, especially the upper part of the human skeleton, which consists of the skull and its parts. Interest was in the vibration behavior of the mandible, as understanding how the mandible reacts to vibrations may have important implications for patient treatment in various medical situations, such as postoperative recovery, wound healing, or standard dental procedures. For example, vibrations may affect the blood flow, tissue regeneration, pain perception, or bone density of the mandible. Therefore, we aimed to investigate the vibration behavior of the mandible using a 3D model and frequency analyses.

This paper presents the results of an investigation of the vibration behavior of the mandible. A 3D mandible model was developed from CT scans and refined for the analysis. We performed frequency analyses of the model using material properties (Young's elasticity modulus and Poisson's ration) and boundary conditions that were adapted from the literature. As the result of the analysis, the natural frequencies for the first ten modes were determined.

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.

These instruments may induce high-frequency resonance in the mandible, which may cause discomfort, damage, or fracture. We analyzed the resonance frequencies and modes of the mandible, and discussed their significance for the vibration response and the dental treatment.

Acknowledgement:

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S02: Biomechanics

Organizer(s): Budday, Silvia *(Friedrich-Alexander-Universität Erlangen-Nürnberg)*
Linka, Kevin *(RWTH Aachen University)*

S02.01: Bone and aneurysms

Date: March 19, 2024 08:30–10:30
Room: G22/111
Chair(s): Linka, Kevin

Finite Element Modelling of Concentrated Impact Loads on the Masticatory Muscles at the Head

Wang, Zechang (1); Behrens, Roland (1); Elkmann, Norbert (1); Juhre, Daniel (2) 08:30
1: Fraunhofer IFF
2: Otto von Guericke University Magdeburg

Numerical simulation has great potential to provide a more comprehensive understanding of human impact response to injury mechanisms. Finite Element (FE) models are used as a tool to study human injuries in greater detail, e.g. the THUMS model, which is widely used as a reliable human model in different fields and can be used to predict human injuries such as fractures, internal organ damage, brain tissue injuries. However, no available FE model can be used to simulate human-robot collisions based on standards ISO 15066 and the biomechanical characteristic of human soft tissues in vivo.

The authors have developed a head model based on the structures (dimensions and anatomy) of the THUMS head model, specifically designed to simulate impact loads on the masticatory muscles. Based on medical imaging (MRI) data, the soft tissues at the location of the masticatory muscles in the THUMS head were transformed from monolayer to multilayer, i.e., a composite geometry of skin-fat-muscle each with its own material model and parameters. The experimental data from the Fraunhofer IFF living subjects study were used to optimize and validate this model. The objective of the Fraunhofer IFF study was to determine biomechanical thresholds for a specific set of body locations in ISO 15066 under dynamic collisions.

Using this model, the dynamic collision from different rigid bodies, especially the robot's part on the masticatory muscles, can be simulated under the limiting effect of pain onset. The simulation results represent the real biomechanical response of the soft tissues in the head in vivo under external loading.

Identifying a suitable material model to simulate the implantation process of endoprostheses into human bone

Strackeljan, Cornelius; Duvigneau, Fabian; Woschke, Elmar 08:50
Otto von Guericke University Magdeburg

Modern shoulder arthroplasties with stemless implants help to preserve larger parts of the original bone substance and to reduce potential risks of conventional implants. Their shape allows newly formed bone
structures to grow directly through the implant. However, it is not fully explained how an optimal fixation of the implant by formation of new bone can be achieved or stimulated.

In this context, we develop a method to simulate the mechanical loading in the humerus during the operation using the finite element method. The calculation results will be used to investigate whether one or more mechanical stress variables, e.g. stresses or elastic/plastic strains, can be correlated with measurement data of cell activity in the bone, which is available in the form of SPECT/CT data.

Up to now, a very simple material model has been used for the simulation. This contribution explores the suitability of other, more sophisticated material models. Experimental data, which were collected using humeral heads from shoulder surgeries at the University of Magdeburg serve as a basis for this investigation.

On the application of the Finite Cell Method to static analysis of trabecular bone tissue specimen using high-resolution microCT data

Shahmohammadi, Mohammad Amin (1); Fiedler, Imke (2); Busse, Björn (2); Düster, Alexander (1) 09:10
1: Hamburg University of Technology
2: University Medical Center Hamburg-Eppendorf

This study aims to introduce a robust numerical approach to simulate complex small-scale mediums such as trabecular bone tissue in form of a cylindrical specimen taken from human vertebra. Consideration of previous related studies indicates that there are several challenges in utilizing standard finite element (FE) techniques for analysis of such biomechanical structures. This is mainly due to their time-consuming numerical procedure required for generating geometry conforming meshes. In this regard, the Finite Cell Method (FCM) is an interesting alternative because it is based on the concept of the fictitious domain technique in which underlying meshes do not need to conform to the boundary of the domain. Since the considered trabecular bone tissue consists of a complex small-scale internal morphology, generating a FE mesh is rather complicated. So, the application of the FCM can be justified by overcoming the mentioned shortcomings of FE methods for this problem. Using FCM, it is possible to simulate the mentioned vertebra tissue cylindrical specimen using higher order cells of regular shapes where the geometry is taken care of through the numerical integration. The input for the present numerical tool corresponding to the complex internal morphology of the proposed tissue is given by a high-resolution microCT scan. The outcome of the FCM will be compared to results obtained by mechanical testing of the specimen.

Numerical simulation of individualized flow diversion cerebral aneurysms treatment

Do, Huy Quang (1); Juhre, Daniel (1); Makvandi, Resam (2); Ding, Andreas (2) 09:50
1: Otto von Guericke University Magdeburg
2: Acandis GmbH, Germany

Flow diverter implantation has become an established treatment of cerebral aneurysms over last ten years. However, a flow diverter treatment always requires detailed patient specific planning as complications can arise with the available standard devices. To overcome this challenge, the use of robust predictive simulation tools is necessary to assist and optimize the intervention procedure. The aim of this study is to develop a design tool for numerical simulation of flow diverter in crimping and navigating processes.

Mechanical behaviours of a braided flow diverter under crimping contact interaction by a catheter are simulated using LS-dyna software. The deformed shapes of the flow diverter wires are computed using an IGA discretization of beam elements with a pseudo-elasticity of shape memory alloy material model. Then, the crimped flow diverter in a catheter is navigated through a patient specific blood vessel to the position of the aneurysm. In this navigation process (modelled by Grasshopper within Rhinoceros3D CAD software), the flow diverter at first is aligned along the central axis of the blood vessel, then in the next step it is moved along this central axis. The challenge lies in the fact that the crimped flow diverter ideally moves mainly in a translatory manner and does not twist too much. Therefore, the central axis is optimised to ensure that there are no sudden changes in curvature to avoid severe torsions. This design tool serves as a basis to expedite design development prior to prototype manufacturing.

Sensitivity study of a computational model for endovascular coil deployment in cerebral aneurysms

Holzberger, Fabian; Muhr, Markus; Wohlmuth, Barbara 10:10
Technical University of Munich

Endovascular coil embolization is one of the primary methods for the treatment of a ruptured or unruptured cerebral aneurysm. Although it is a well established and minimally invasive method, it bears the risk of suboptimal coil placement, which can lead to incomplete occlusion of the aneurysm, causing in the worst case even aneurysm recurrence. Our study investigates factors that lead to a

suboptimal placement when a coil is deployed in an aneurysm. To this end, we use a mathematical model that simulates the embolization process of the coil in patient specific three-dimensional aneurysm geometries.

One of the key features of coils is that they have an imprinted natural shape which supports the fixation within the aneurysm. We account for the latter property by introducing bending and torsional forces into our model of the coil. This enables the placement of multiple coils with different natural shapes in an aneurysm, as it is done in real interventions. In order to differentiate optimal from suboptimal placements, we employ the Raymond–Roy occlusion classification and measure the local packing density in the aneurysm at its neck, wall-region and core. We take uncertainties, e.g., in the material parameters, position- and angle of insertion into account by running for each placement several simulations with variations in the setup, allowing us to average their local packing densities.

Our mathematical model of the coil is based on the Discrete Elastic Rod model which is a dimension-reduced 1D PDE system taking into account bending and twisting response such as its natural curvature. Collisions between coil segments and the aneurysm-wall are taken into account by an efficient contact algorithm that is based on an Octree collision detection. The numerical solution of the model is obtained by the semi-implicit Euler time stepping method. Our model can be easily incorporated into blood-flow simulations of embolized aneurysms.

S02.02: Constitutive modeling

Date: March 19, 2024 16:30–18:30
Room: G22/111
Chair(s): Balzani, Daniel

A Thermodynamic framework for constructing a constitutive model accounting for fiber reorientation through active and passive responses

KUMAR, RAHUL 16:30
Indian Institute of Technology Madras, India

In the scientific literature, “remodelling” means a reorientation of the internal microstructure of materials. This change is achieved by reorganizing existing constituents, such as altering their orientation, cross-linking, or synthesizing new constituents with a different organization. Remodelling may or may not alter the mass density, but it does impact other material properties like stiffness or symmetry Humphrey and Rajagopal (2003). Among the different forms of remodeling, this discussion focuses on the reorientation phenomenon observed in fiber-reinforced biological tissues, exemplified by structures like the aorta, which showcase their transversely isotropic nature—where a predominant direction influences mechanical behavior.This work pioneers a mechanical model for anisotropic materials possessing three independently evolving fiber families, allowing for active reorientation mechanisms influenced by external forces and internal material changes. The evolution equations are derived in a thermodynamically consistent way, and passive and active contributions to the reorientation process are identified. Using experimental data from existing literature, our research demonstrates that the proposed model accurately aligns with experimental findings regarding fiber orientation, encompassing both constrained and unconstrained fiber evolutions. Despite the primary focus on biological applications, our framework holds broader applicability. It can be readily adapted to describe engineering materials, such as composites featuring four families of fibers engineered to reorient under distinct stimuli. This versatility indicates its potential for various material science applications beyond biological contexts.

Constitutive Modeling of Viscoelastic Behavior and Irreversible Damage in Porcine Pulmonary Artery

Reddipaga, Mani (1); Kannan, Krishna (1); Baek, Seungik (2) 16:50
1: Indian Institute of Technology Madras, India
2: Michigan State University, USA

Pulmonary hypertension (PH) is a cardiovascular condition associated with elevated pulmonary arterial pressure. Evidence from animal studies shows that the irreversible process of pulmonary arterial wall damage plays a significant role in disease progression. In the present study, we apply the thermodynamic framework of multiple evolving natural configurations to develop a constitutive model to describe the nonlinear viscoelastic behaviour and irreversible damage of the porcine pulmonary artery over finite strains. The permanent set (irreversible deformation) of the tissue, when loaded beyond a certain physiological range, is a manifestation of structural damage to the tissue. Motivated by the one-dimensional rheological model, we develop a three-dimensional viscoelastic-plastic model for finite deformations. As a part of the framework, we choose specific forms for the strain energy potential and the rate of dissipation. The dissipation is additively decomposed into contributions from the viscous and plastic behaviour. The requirement of homogeneity on the latter, together with the reduced energy equation, leads to yielding behaviour. The final constitutive equations are obtained by maximizing the rate of dissipation subjected to the reduced dissipation inequality and the incompressibility constraint. The model's efficacy is tested with the inflation-extension data of a porcine pulmonary artery. The model predicts a progressively increasing permanent set with subsequent pressure cycles consistent with the observed values.

Fast simulation of coronary in-stent restenosis: a non-intrusive data-driven reduced order surrogate model

Shi, Jianye; Manjunatha, Kiran; Reese, Stefanie 17:10
RWTH Aachen University

The intricate process of coronary in-stent restenosis involves the interplay between different mediators, including the platelet-derived growth factor (PDGF), the transforming growth factor-β(TGF-β), the extracellular matrix (ECM), the smooth muscle cells (SMC), and the drug elution from the stent. Modeling of such complex multiphysics phenomena demands extensive computational resources and time. Reduced order surrogate models serve as a compelling alternative to the comprehensive full-order model. This paper proposes a non-intrusive data-driven reduced order modeling approach for the underlying multi-query time-dependent parametrized problem. In the offline phase, a 3D convolutional autoencoder, comprising an encoder and decoder, is trained to achieve dimensionality reduction. The encoder condenses the full-order solution into a lower-dimensional latent space, while the decoder facilitates the reconstruction of the full solution from the latent space. To deal with the 4D input data (3D geometry + 1D time series), two ingredients are explored. The first approach incorporates time as an additional parameter and applies 3D convolution on individual time-steps, encoding a distinct latent variable for each parameter instance within each time-step. After training, dynamic mode decomposition (DMD) is addressed to continuously span these latent variables across the time-domain. The second approach reshapes firstly the 3D results into 2D along a less interactive axis and stacks all time-steps in the third direction for each parameter instance. This rearrangement generates a larger and complete data-set for one parameter instance, resulting in a singular latent variable across the entire time-series. Gaussian process regression (GPR) is then used to establish correlations between the latent space and the input parameters. Comparative analysis are conducted to discern the limitations, advantages, efficiency, and accuracy of both methods.

Constitutive Artificial Neural Networks (CANNs): A framework for inelastic anisotropic soft biological tissues

Linka, Kevin (1,2); Abdolazizi, Kian P. (2); Cyron, Christian J. (2,3) 17:30

1: RWTH Aachen University
2: Hamburg University of Technology
3: 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 elastic and inelastic mechanical behavior.

Towards Using Active Learning Methods for Human-Seat Interactions To Generate Realistic Occupant Motion

Fahse, Niklas (1); Harant, Monika (2); Obentheuer, Marius (2); Linn, Joachim (2); Fehr, Jörg (1) 17:50

1: University of Stuttgart
2: Fraunhofer ITWM

Runtime-efficient human active models (RHAM) are a tool to predict human behaviors in static and dynamic driving scenarios, e.g. pre-crash situations. With RHAMs, we want to close the gap between passive Finite Element (FE) and inverse multibody system (MBS) models, especially in situations where the human-machine interaction is at the core of our study.

This contribution uses an MBS modeling approach with active musculature – combined with discrete mechanics and optimal control for constrained systems (DMOCC) [1] – which shows promise for predicting human-like motion [2] without the need of a priori volunteer tracking in experiments.

In the context of occupant motion, the human model is in continuous contact with the vehicle interior, primarily with the vehicle seat. To investigate active behavior with the DMOCC setup in this environment, it is necessary to efficiently evaluate the interaction with the seat. For this purpose, the contact is approximated by a surrogate model using machine learning methods. This not only provides a contact model that can be quickly evaluated, but – with the right class of surrogate – also allows efficient gradient-based methods to be used to solve the optimal control problem.

The surrogate model is created in an offline phase and used in an online phase to model the human-seat interaction in optimally controlled multibody simulations. In the offline phase, the contact is investigated with detailed parameterized FE simulations. Based on the FE human-seat interaction which depends on the parameter sampling, a surrogate model is created using, e.g., an MLP regressor. In the subsequent online phase, occupant movements are investigated in studies in which the human model is in contact with the vehicle seat.

A key challenge is the choice of the training samples, i.e. simulations in the offline phase. Here, transient FE simulations must be performed so that the properties of the contact partners are adequately represented in the training data. To overcome the curse of dimensionality in the parameter space, this contribution proposes an active learning [3] methodology, where in an iterative process new training data is requested for relevant contact situations. These relevant contact situations are generated by

using the preliminary model in the optimally controlled MBS simulations. The resulting overall model is an example of a multiscale model which combines properties from detailed FE and MBS modeling approaches.

[1] Leyendecker et al., Optim. Control Appl. Methods, 2010.

[2] Roller et al., ECCOMAS, 2017.

[3] Settles., UW–Madison, 2009.

S02.03: Multi-body dynamics

Date: March 20, 2024 08:30–09:30
Room: G22/111
Chair(s): Woschke, Elmar

The effect of active leg swing on walking template model dynamics

Renjewski, Daniel 08:30
TU Munich, Germany

The simplest models of bipedal walking concentrate the entire system's mass in one point and, for simplicity, ignore the dynamics of the swing leg. Given the challenges of leg swing in human walking, we will revisit this omission and analyze the impact of its inclusion into our model. We will extend the inverted pendulum model to feature a distributed mass, including masses at the end of each leg. This model has already been used to enhance the motion planning for a bipedal robot.
Swinging the leg forward is a rapid process involving high forces due to rapid accelerations of fairly heavy masses. Observing implementations of swing leg control in technical devices, which is frequently an afterthought for controller development, the realization often uses hip power and, thus, due to the reaction torque on the upper body, has a direct impact on global gait dynamics. The swing leg is also described as causing unwanted yaw torques, which need to be actively compensated for.
Given the facts that human legs account for about 30 % of total body mass, swing forward in a very short period in human walking, and touch the ground with well-matched speed, which has long been mimicked in robots, a conundrum arises, namely why does a model which does not capture swing leg dynamics represent the global dynamics of walking that well? In this work the swing leg dynamics are analyzed and the coupling of swing leg and remaining body investigated based on experimental data and supported by a reductionist three mass model. I aim to show that the proposed model for the swing leg dynamics of Mochon and McMahon matches the real dynamics fairly well and relates it to our previous work for generating the initial impulse to propel the leg into swing.

The analysis demonstrates that the influence of the swing leg cannot be categorically neglected given its substantial mass, high required accelerations, and power draw to accomplish leg swing in the short amount of time during SSP. Considering the power requirements for a successful leg swing, it becomes evident that it is crucial to identify the correct power source for leg swing in human-like walking. This makes the excellent match of global dynamics between human walking and simple models without a swing leg somewhat puzzling. Based on this observation, we can hypothesize that the swing leg seems to be partially decoupled from the rest of the body during swing phase and its actuation during final stance.
A mechanism that can achieve this has been proposed. We postulated an alleviation phase, during which the leg no longer supports the body weight, and the dynamic coupling between the trailing - soon to be swinging - leg and the rest of the body is broken. Our analysis does provide a further indication as it seems that the rapid unloading of the ankle joint and the subsequent leg swing does not have a significant dynamic echo in the global dynamics of the remaining body.

Model Order Reduction of Collision Models for Safe Human-Robot Collaboration

Leinert, Emmely (1); Behrens, Roland (2); Woschke, Elmar (1) 08:50
1: Otto von Guericke University Magdeburg
2: Fraunhofer IFF

Production can be made more efficient and flexible when humans and robots interact. Robots can take on repetitive or ergonomically inconvenient tasks while the human worker can focus on cognitive work. When using a collaborative robot system, contact between human and robot is allowed. Safety requirements and protective mechanisms specified by the technical specification DIN ISO/TS 15066 are required in order to ensure the human's safety. the risk of a robot collision at defined body points can be evaluated by force and pressure limit values. The measurement of force and pressure values requires a biofidel device. Limited accuracy and reliability of the available measuring devices, as well as the time and costs involved in the manual use, have motivated researchers to develop simulative models. These allow the calculation of different contact situations between humans and robots and could replace manual testing in the future.

The aim of this work is to individually adapt a patented biomechanical model (Fast Response Model) developed at the Fraunhofer IFF for selected body parts on the hand-arm system. Furthermore, the focus is on the efficient calculation of the reaction force in an event of a collision between a contact body of any shape and one of the selected body parts. A comparison of the results to those of existing finite element reference models serves to evaluate the plausibility of the model's system response. In addition, the simulation times of the model are compared with those of established models for simulation-based risk evaluation of robot collisions. The model's quality is checked by using a validation geometry.

The results show that depending on the selection of the body part, the end effector geometry and a given displacement, similar results to a finite element model can be calculated. The simulations with the Fast Response Model are, however, less time consuming.

A further topic for continuing work is the use of artificial intelligence. The model could be transformed into a data-driven model that delivers results in real time using machine learning.

Determination of the mechanical properties of the sacroiliac joint of a dog by imaging measurement methods and model update in a multi-body model

Daniel, Christian (1); Burkhardt, Sarah (1); Röhrmann, Nicole (2); Wagner, Franziska (2); Woschke, Elmar (1) 09:10
1: Otto von Guericke University Magdeburg
2: Leipzig University

The sacroiliac joint (SIJ) is the articulated connection between the sacrum and the ilium and is a tight, combined, and only slightly mobile joint. In many dogs, the joint becomes stiff with age. As a result, the animal experiences pain while moving. Too little information is known about the degree of stiffening and the physiological range of motion for therapy. Consequently, recording the range of motion of different individuals (healthy and diseased) is a step towards a better understanding of sacroiliac syndrome. For the basic investigation of the mechanical properties of the SIJ, post-mortem examinations should be performed on different individuals. To determine the mobility of the joint, the sacrum is fixed and a movement is forced on the ilium using actuators. The forces required for this are recorded. In addition, the spatial movement of the ilium and sacrum is recorded. The kinematic and dynamic variables can be used to determine the translational and rotational stiffness of the SI

joint. As it is not possible to apply directed loads to the ilium, the measurement data is used to determine the elastic parameters of the joint ligaments using heuristic methods. The multi-body model includes the ilium, the ligaments and the actuators of the test stand with their spatial orientation.

S02.04: Mechanical testing and parameters

Date: March 20, 2024 14:00–16:00
Room: G22/111
Chair(s): Shi, Jianye

Multiscale Analysis of Human Dura Mater – From Nano- to Macroscale

Niestrawska, Justyna Anna (1); vom Scheidt, Annika (1); Liprandi, Daniele (2); Rodewald, Marko (3,4); Hammer, Niels (1,5,6)

1: Medical University of Graz
2: University of Greifswald
3: Leibniz Institute of Photonic Technology
4: Leibniz Center for Photonics in Infection Research
5: University of Leipzig
6: Fraunhofer IWU

14:00

The outermost layer of the meninges, known as the dura mater, forms a protective membrane around the brain and spinal cord. Composed of dense and fibrous connective tissue containing collagen and elastin fibers, proteoglycans, and other extracellular matrix components, the dura mater plays a crucial role in upholding the stability and integrity of the central nervous system. Additionally, it regulates cerebrospinal fluid dynamics, safeguarding neural tissue from mechanical stress and injury. Despite its significance in the context of conditions like traumatic brain injury, computational and physical human head models often ignore the dura mater. To date, biomechanical tests have not provided insights into the anisotropic mechanical characteristics of different regions of the human dura mater under physiological conditions. Moreover, there is insufficient comprehensive quantification of the orientation of collagen fibers, contributing to a limited understanding of this aspect. Consequently, our aim was to investigate the characteristics of collagen on the nano- to macroscale in the human dura mater under multi-axial loading.

In a first study, the mechanical and structural anisotropy of different regions of the human dura mater was mapped. Mechanical data was correlated with the quantification of collagen fiber orientation. The collagen microstructure of samples from four donors was analyzed utilizing second-harmonic generation imaging. The macroscopic mechanical behavior was investigated by subjecting sixty samples from six donors to quasi-static, uniaxial tension tests until failure in a heated tissue bath. For this, a Z020 torsion multi-axis testing system (ZwickRoell AG, Ulm, Germany) together with an Aramis image correlation system (GOM, Braunschweig, Germany) was used.

Further, possible sex-dependent alterations in nanostructure and its influence on macroscopic biaxial mechanical properties induced by ageing were investigated. Square samples (15 × 15 mm²) were subjected to biaxial loading with simultaneous microfocussed ultra-small-angle X-ray scattering to determine changes in collagen fiber orientation and d-spacing with deformation (MiNaXS beamline P03/PETRA III, DESY).

The obtained data shed light on nano- to macroscale mechanisms and were utilized to determine the failure stress and strain, E-moduli, and a microstructurally motivated material model was employed to examine local differences in both structure and mechanics. Significant differences in collagen fiber dispersion and main fiber orientation were found between the locations. Although structural parameters for the material model were only available for four out of six donors, the resulting parameter set resulted in good fitting results, providing a more detailed understanding of collagen characteristics of the human dura mater.

Seasonal variation of Elymus for the assessment of ecosystem services

Liu, Jintian; Liu, Qiyue; Kutschke, Steven; Kosmalla, Viktoria; Schürenkamp, David; Goseberg, Nils; Böl, Markus
TU Braunschweig

14:40

Heavy wave action can lead to sedimentation, with soil material being transported seawards. The potential for erosion and sedimentation increases with wave height and flow rate. If the coastal region is exposed to long-term fluctuations and cannot be restored to its original state, the shoreline will retreat landwards, resulting in damaging conditions, including global sea level rise and threatened coastal properties. Native vegetation plays an important role in protecting the coastal areas from erosion. On the one hand, the plants bind and secure the soil, which helps to improve the stability of the coastal region, and on the other hand, the plants on the foreshores have great influence on the flow patterns and velocity profiles. Elymus is one of the most important plants for ecosystem services. With this in mind, the mechanical behaviour of Elymus has been experimentally characterised to gain a better understanding of the bending flexibility of the plants and the wave-plant interaction, as well as their contribution to wave energy dissipation and erosion control.

In order to investigate the seasonal variation in mechanical behaviour, three-point and two-point bending experiments were performed on Elymus in relation to different seasons (March, June, September) and stem sections (bottom, middle, top). The aim was to determine both the structural and material properties of Elymus and to investigate the comparability between the different time points. To this end, tissue-specific histological studies were performed on stem cross-sections, from which the material properties were derived from the structural behaviour using the inverse finite element method coupled with a non-linear material model. The experimental results show significant differences in the bending stiffness of the stem cross-sections with respect to different sampling times. In addition, the histological and numerical results provide useful information about the stem geometric and material properties in different seasons, which can be used numerically to predict the wave-plant interaction as well as the resulting wave properties in dependence on different configurations, such as plant stiffness, plant cross-sectional dimension, and plant density.

Location and layer-dependent biomechanical characterization of the porcine small intestine wall

Hasselbeck, Dorina; Liu, Jintian; Böl, Markus
TU Braunschweig

15:00

Gastrointestinal perforations (GIPs) are medical emergencies resulting from a direct mechanical injury or progressive damage to the bowel wall due to various underlying conditions. The former occurs as a result of blunt trauma or puncture during medical procedures, while the latter may be due to the infection or patient obstruction. GIPs pose a risk by allowing intestinal contents and bacteria to enter the abdominal cavity, potentially leading to serious complications such as peritonitis or abscess. Understanding the microstructure and mechanical behaviour of the intestinal wall is crucial to understanding of the loss of organ stability. Against this background, this study aims to experimentally investigate the layer-specific mechanical behaviour of the small intestinal wall (SIW) and to generate data for the development and validation of a material model describing the formation of GIPs. For this purpose, single-notched tensile tests, peeling tests, and biaxial tests were performed on the porcine SIW. Starting from the non-failure behaviour characterised by biaxial tensile tests, the interlayer failure behaviour of the SIW is characterised by single-notched tension tests on each layer with respect to different organ sections and orientations, taking into account the multi-layer and fibre-oriented structure. In addition, the interfacial failure behaviour is characterised by peeling tests.

The results show different mechanical behaviours between the SIW layers, highlighting different failure characteristics. Anisotropic material behaviour occurs in all layers and in the SIW. In addition, the analysis of non-failure behaviour provides valuable information on how the SIW responds under biaxial loading conditions, which more accurately replicates the *in vivo* situation compared to uniaxial tests. Overall, the layer-specific properties obtained provide important critical mechanical data and

have the potential to improve surgical techniques and medical device designs. Furthermore, the results could aid in early diagnosis and treatment by providing information for numerical prediction of GIPs.

On the morphological and mechanical properties of filamentous pellets along the culture process

Liu, Qiyue; Liu, Jintian; Kozanecka, Zuzanna; Krull, Rainer; Böl, Markus 15:20
TU Braunschweig

Filamentous bacteria and fungi are important producers of pharmaceutical compounds. Among them, Actinomadura namibiensis has been received more attention for this ability to produce the secondary metabolite labyrinthopeptin A1, a type of lantibiotic featuring with antiviral activity against HIV, HSV, Dengue, and Zika viruses. The preliminary work showed that the production of labyrinthopeptin A1 is influenced by the culture medium, the culture process, the pellet morphology, and the pellet material behaviour. For example, a dense pellet structure does not show an advantage for the transport of the substance within the pellet. In addition, the preliminary work has shown that the productivity is positively correlated with contact energy during the shaking process. Taking all these contributions into account, the whole cultivation process can be divided into two main stages. In the initial stage, both biomass and pellet size increase rapidly, associated with an obvious decrease in glucose and soluble starch. During the steady state, the maximum productivity is reached just before the glycerol and carbohydrate sources are exhausted.

In order to gain a better understanding of the growth mechanisms of pellets and to optimise the cultivation process with increasing productivity, the pellets were experimentally characterised using a micromechanical setup. Since pellets have an irregular geometry, with tightly interlaced and branched filament networks, pellet-specific mechanical experiments were performed with respect to different pellet dimensions and cultivation times using the slice sampling method, taking into account the morphological changes during the culture process. In addition, size distributions of pellets were obtained by optical microscopy and collected over the cultivation time. Based on the force-displacement relations and the digitally recorded pellet-specific geometry, the correlation between mechanical behaviour and structural properties will be determined along the whole culture process. The force response to cyclic loading is mainly dominated by elastic behaviour, while the slight force decrease at maximum loading contributes to the small plastic deformation of the pellets. Material parameters can be derived from the measured force-displacement relations and further substituted into the contact model to describe the pellet interactions during the shaking process, which helps to numerically predict the culture process under different configurations, such as shaking speed, pellet seeding density.

Global sensitivity analysis for biomechanical models with dependent input parameters

Brandstaeter, Sebastian; Popp, Alexander 15:40
University of the Bundeswehr Munich

A significant source of uncertainty in predictions of sophisticated mechanistic models results from a lack of knowledge about their numerous parameters. Achieving patient-specific measurements for all parameters is impractical. Thus, a strategic focus on the key parameters driving most of the predictive uncertainty becomes imperative.
Our recent work demonstrates the indispensability of variance-based global sensitivity analysis using Sobol indices in identifying influential and uninfluential parameters in complex biomechanical models [1, 2]. However, a notable limitation arises from the method's assumption of parameter independence. This assumption is problematic for many biomechanical models where such independence does not hold. In response, we demonstrate a global sensitivity analysis method that overcomes this restriction [3]. We showcase the properties and capabilities of the method through examples, illustrating how it assesses the contributions of the potentially dependent parameters to the predictive uncertainty of in silico models of biological systems. In summary, the presented framework provides a robust tool that extends the concept of global sensitivity analysis to a broad class of biomechanical models, particularly those with dependent input parameters.

[1] Brandstaeter S., Fuchs S. L., Biehler J., Aydin R. C., Wall W. A., and Cyron C. J. (2021) 'Global Sensitivity Analysis of a Homogenized Constrained Mixture Model of Arterial Growth and Remodeling', J. Elast., 145(1–2), pp. 191–221. doi: 10.1007/s10659-021-09833-9.

[2] Wirthl B., Brandstaeter S., Nitzler J., Schrefler B. A., and Wall W. A. (2023) 'Global Sensitivity Analysis Based on Gaussian-Process Metamodelling for Complex Biomechanical Problems'. Int. J. Numer. Meth. Biomed. Eng., 39 (3): e3675. doi: 10.1002/cnm.3675.

[3] Bertrand I., and Prieur C. (2019). 'Shapley Effects for Sensitivity Analysis with Correlated Inputs: Comparisons with Sobol' Indices, Numerical Estimation and Applications'. Int. J. Uncert. Quantif., 9 (5): 493–514. doi: 10.1615/Int.J.UncertaintyQuantification.2019028372.

S02.05: Brain

Date: March 20, 2024 16:30–18:30
Room: G22/111
Chair(s): Budday, Silvia

Using active learning and surrogate models in the inverse viscoelastic parameter identification of human brain tissue

Hinrichsen, Jan (1); Ferlay, Carl (2); Reiter, Nina (1); Budday, Silvia (1) 16:30
1: FAU Erlangen-Nürnberg
2: École polytechnique, France

Inverse mechanical parameter identification is crucial for characterizing ultrasoft materials under inhomogeneous deformation. However, the process is often computationally expensive, primarily due to the complexity of the forward model. While simulation methods like finite element models can handle intricate geometries and implement complex constitutive equations, they come with high computational costs. To address this challenge, data-driven machine learning models, specifically neural networks, can serve as efficient surrogate models, replacing the need for complex high-fidelity simulations.

In this approach, neural networks act as reduced-order models post an initial training phase, during which they learn the relationships between inputs and outputs of the high-fidelity model. Generating the necessary training data is computationally expensive due to required simulation runs. Active learning techniques play a crucial role by identifying strategically valuable training points that contribute significantly to the accuracy of the trained model.

In this study, we introduce a recurrent neural network capable of effectively approximating the output of a viscoelastic finite element simulation, substantially reducing evaluation times. Additionally, we leverage Monte-Carlo dropout-based active learning to pinpoint highly informative training data. To demonstrate the efficacy of our developed pipeline, we apply it to the identification of viscoelastic material parameters for human brain tissue.

Modeling the porous properties of brain tissue

Greiner, Alexander (1); Comellas, Ester (2); Steinmann, Paul (1); Budday, Silvia (1) 16:50
1: FAU Erlangen-Nürnberg
2: Universitat Politècnica de Catalunya, Spain

The porous properties of brain tissue remain poorly understood and their investigation requires profound experimental setups and modeling approaches. Computational models based on the theory of nonlinear continuum mechanics have proven to be a valuable tool to understand the physical mechanisms underlying the tissue response and can assist a profound analysis of associated experimental data. Through numerical experiments, we identified a strong coupling between the volumetric response of the solid matrix and the porous effects in our nonlinear poro-viscoelastic model, thus, making material parameter identification even more challenging.

To investigate the influence of porous contributions to the tissue response under different loading conditions, we model brain tissue as a poro-viscoelastic material using a numerical framework based

on the Theory of Porous Media. The underlying strain-energy function possesses an extension function to capture the compaction point, i.e., when all fluid has left the tissue. The associated volumetric stress contribution depends on the initial solid volume fraction, the Jacobian of the biphasic material and is scaled by the first Lameṕarameter. Therefore, low values of the first Lamé parameter lead to a gradual increase of the volumetric stress response towards the compaction point. In contrast, high values of the first Lamé parameter lead to an immediate, strong volumetric response – even for small volumetric changes. In fact, the overall biphasic tissue response is highly sensitive to the choice of the first Lamé parameter, and, high values of the first Lamé parameter obliterate the porous effects such that our biphasic model acts like an incompressible solid model – independent of the permeability.

For low values of the first Lamé parameter, we observe that a poroelastic one-term Ogden model, i.e. without viscosity, captures two important characteristics of brain tissue, relaxation and hysteresis – highlighting the importance of porous effects in brain tissue. We will further show the influence of the first Lamé parameter on the material parameters identified through an inverse parameter identification scheme. Eventually, we will discuss possibilities to incorporate these insights into the design of new experimental setups, focusing on the identification of the first Lamé parameter and the intrinsic permeability.

A constitutive relation for human brain tissue obtained using an inverse technique and the numerical study of existence of non-classical solutions

Das, Mrunal Kanti; Kannan, Krishna 17:10
Indian Institute of Technology Madras, India

A proper understanding of the mechanical behaviour of human brain tissue is crucial for studying traumatic brain injuries such as concussions or impact-related injuries. It helps in surgical planning and simulation by revealing how brain tissue deforms and responds to surgical interventions. The human brain tissue exhibits complex responses in shear-superposed uniaxial deformations, demanding an intricate mathematical structure of the constitutive relation. This requires developing a novel methodology to construct a unique mathematical form of the stored energy for any isotropic incompressible hyperelastic material subjected to shear superposed on uniaxial deformation. We introduce an inverse technique, which uses the shear stress data in the homogeneous combined tension/compression and shear experiment as an input. Accordingly, the shear stress functional form is assumed to be known. The other unknown components of stress are systematically determined by using the universal relation, boundary conditions, and the existence of the stored energy. Incorporating Lode invariants of Hencky strain in the inverse procedure, instead of principal invariants, simplifies the integration of the resulting partial differential equation for the existence of stored energy. This facilitates the derivation of a concise two-parameter hyperelastic constitutive relation for human brain tissue. The ABAQUS implementation, utilizing UHYPER and VUMAT subroutines, effectively captures a comprehensive range of both classical and non-classical solutions inherent in physical deformations. The barrelling-dominated and buckling-dominated solutions of a solid cylinder subjected to axial compression and the creasing solution captured on compression of a cuboid show the constitutive model's robustness and richness of solutions. The prospective development of current constitutive models will be crucial for advancing computational models simulating brain biomechanics in complex deformations.

Construction of a Hyperelastic Potential for human brain tissue using an Inverse Method and its Finite Element Implementation to study 3D Boundary Value Problems

Vaidya, Yagnik Kalpeshkumar; Kannan, Krishna 17:30
Indian Institute of Technology Madras, India

Understanding the mechanics of the human brain is crucial to understanding various avenues such as injuries from impacts, surgery planning, the response of the brain to medical treatments, and the mechanical aspects of disease progression. Hence, an accurate description of the complex mechanical response of the human brain tissue is necessary and requires sophisticated modelling techniques. We construct a potential energy function using a novel inverse procedure wherein the shear response

is taken as input from the experimental data. The combined application of universal relation, boundary conditions, and the existence of stored energy uniquely determines the remaining components of stress and, consequently, the mathematical form of the stored energy. Using Lode invariants of the Hencky strain facilitates analytical integration of the response function to derive the stored energy. The model is implemented in ABAQUS using the UHYPER subroutine. The simulation results correspond well with the experimental data of shear superposed on uniaxial deformation reported in Budday et al. (2017). However, the material parameters which are determined based on the assumption of homogeneous deformation yields significantly different results for the full-field problem. This observation questions the commonly employed validity of the assumption of homogeneous deformations while determining the material parameters. Consequently, we re-determine the material parameters for the full-field problem by minimizing the differences in the global reaction forces using an evolutionary algorithm in the commercial tool ISIGHT. Using the 'corrected' values, we study various inhomogeneous boundary value problems, such as the effect of the tumour growth on the surrounding brain tissue and capture real-time simulation data.

Coupling of neuronal excitation and mechanosensitive ion channel activation in the human brain

Werneck, Linda (1); Keip, Marc-Andre (1); Ortiz, Michael (2) 17:50

1: University of Stuttgart
2: California Institute of Technology, USA

In the context of ultrasound neuromodulation, mechanical ion-channel activation, ion channel flow, and neuronal activation are strongly interdependent. While the conductance-based Hodgkin-Huxley (HH) model of action potentials and the Poisson-Nernst-Planck (PNP) equations for ion flux both consider different ion species and membrane potentials, their link with regards to mechanosensitive channels is not obvious.

In the present contribution, a model for coupling of the HH model with the PNP equations is presented in a statistical mechanics framework. In the coupling, changes in intracellular ionic concentration, membrane potentials, and mechanical activation of ion channels are considered. Further, results are discussed with regards to experimental in-house data and further insights are given.

S02.06: Arterial and cardiac mechanics

Date: March 21, 2024 08:30–10:30
Room: G22/111
Chair(s): Niestrawska, Justyna Anna

Computer Simulation of Damage, Fiber Realignment, Growth, and Smooth Muscle Activation in Arteries in Health and Disease

Balzani, Daniel 08:30

Ruhr University Bochum

Cardiovascular diseases are among the most common causes of death worldwide, and atherosclerotic arteries, in particular, are often the root of pathogenesis. There is, therefore, a great medical interest in their analysis and in the optimization of diagnostic and therapeutic methods. In this context, computer simulations which require reliable models for the biological tissue in the vessel walls are increasingly being used. Specifically with regard to the adaptive response, recent advances have made the coupled simulation of growth-induced residual stresses, fiber realignment and smooth muscle activation feasible allowing for a realistic representation of arteries under physiological conditions. For supra-physiological loadings, the incorporation of microscopic damage becomes necessary, e.g., when balloon angioplasty is performed. In this context, the recently proposed concept of re-convexification allows the mesh-independent simulation of strain-softening observed in soft biological tissues. Aside from these aspects, the interaction of the tissue with e.g., hypertensive drugs has gained attention in recent years and can be modeled by a suitable extension of smooth muscle models and the incorporation of the related drug perfusion.

Correlative analysis of highly resolved AAA wall composition and strain in mice

Hegner, Achim (1,2); Cebull, Hannah L. (3); Gámez, Antonio J. (2); Blase, Christopher (1,4); Goergen, Craig J. (3); Wittek, Andreas (1)

1: Frankfurt University of Applied Sciences
2: University of Cádiz, Spain
3: Purdue University, USA
4: Goethe University Frankfurt

09:10

1. Introduction

Abdominal aortic aneurysms (AAA) and dissections are degenerative diseases of the aortic wall with characteristic changes in wall microstructure, composition, and elastic properties. *In vivo* full-field strain measurement can provide noninvasive information on the deformation of the aneurysmal wall, which is closely related to the elastic tissue properties. In this study, the *in vivo* strain distributions in a murine aortic dissection model were determined for different arterial wall regions and compared to the tissue composition, identified by histological staining.

2. Materials and Methods

Aneurysm formation was induced in five *apoE*$^{-/-}$ mice by angiotensin II infusion. The 3D *in vivo* wall strain was determined from high frequency 4D ultrasound imaging by use of the direct deformation estimation approach (DDE) [1]. The AAA wall composition at two positions in each aorta was analyzed from histological sections stained with Movat pentachrome [2].

The different components of the aneurysms were manually segmented in the histological images: regions containing elastin with and without thrombus attachment, fragmented elastin, and thrombus with and without red blood cells (RBCs). Finite element (FE) models were built from the individual contours of the histological segmentations which correspond to an unloaded configuration. The inner and outer contours of the aortic wall of each histological section were registered onto the inner and outer contour of the aortic wall from *in vivo* ultrasound imaging. The displacements from the registration were used as boundary conditions in the FE models to find the deformed configuration. Based on these contours, the strains within the different tissue regions were statistically analyzed.

3. Results

3D strain in the media was significantly reduced in wall regions with thrombus attachment and where the elastic lamellae were fragmented (p<0.05). Strain in thrombus regions without RBCs were also significantly reduced compared to regions with RBCs (p<0.05).

4. Discussion and Conclusions

In vivo strain mapping analysis is sensitive to wall composition; both strain amplitude and heterogeneity of the strain distribution depend on wall composition. Interestingly, thrombus with RBCs displayed relatively high strain values compared to other stiffer regions, suggesting that the size, composition, and age of intramural thrombus all influence aortic dissection kinematics.

5. References

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Fast and Reliable Reduced-Order Models for Cardiac Electrophysiology

Chellappa, Sridhar (1); Cansiz, Baris (2); Feng, Lihong (1); Benner, Peter (1); Kaliske, Michael (2)

1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: TU Dresden

09:30

Mathematical models of the human heart increasingly play a vital role in understanding the working mechanisms of the heart, both under healthy functioning and during disease. The ultimate aim is to aid medical practitioners diagnose and treat the many ailments affecting the heart. Towards this, modelling cardiac electrophysiology is crucial as the heart's electrical activity underlies the contraction mechanism and the resulting pumping action. Apart from modelling attempts, the pursuit of efficient, reliable, and fast solution algorithms has been of great importance in this context. The

governing equations and the constitutive laws describing the electrical activity in the heart are coupled, nonlinear, and involve a fast moving wave front, which is generally solved by the finite element method. The numerical treatment of this complex system as part of a virtual heart model is challenging due to the necessity of fine spatial and temporal resolution of the domain. Therefore, efficient surrogate models are needed to predict the electrical activity in the heart under varying parameters and inputs much faster than the finely resolved models.

In this work, we discuss an adaptive, projection-based reduced-order surrogate model for cardiac electrophysiology. We introduce an a posteriori error estimator that can accurately and efficiently quantify the accuracy of the surrogate model. Using the error estimator, we systematically update our surrogate model through a greedy search of the parameter space. Furthermore, using the error estimator, the parameter search space is dynamically updated such that the most relevant samples get chosen at every iteration. The proposed adaptive surrogate model is tested on three benchmark models to illustrate its efficiency, accuracy, and ability of generalization.

Towards Integral Validation Strategies of Active Cardiac Contraction Models

Ogiermann, Dennis (1); Perotti, Luigi E. (2); Balzani, Daniel (1)

1: Ruhr University Bochum
2: University of Central Florida, USA

09:50

Understanding cardiac function is critical to improve clinical treatments for a wide range of cardiovascular diseases. Mathematical models of the human heart can be of great help in supplementing experimental and clinical data by providing a framework to test theoretical hypotheses and investigate which predictions agree or fail to reproduce observed findings. For example, models are tested against their ability to reproduce pressure-volume loops and the mechanism behind the Frank-Starling effect. However, these models usually fail to reproduce another important validation criterion, i.e., the experimentally observed global and local strain patterns. This raises the question about the origin of the strain discrepancy, while pressure-volume loops are correctly reproduced. A better understanding of the mechanisms leading to the observed cardiac strains will aid in developing a better understanding of cardiac function and, associated to this, heart failure and cardiac remodeling. As a first step in addressing this question, we will show an investigation of geometrical and structural aspects of idealized ventricular geometries with an extended Hill framework, which allows a unified analysis of most of the existing cardiac contraction models.

S02.07: Multi-scale modeling

Date: March 21, 2024 14:00–16:00
Room: G22/111
Chair(s): Lambers, Lena

Immersed boundary approach for vascularized tissues

Belponer, Camilla (1,2); Caiazzo, Alfonso (2); Heltai, Luca (3); Müller, Lucas O. (4)

1: University of Augsburg
2: Weierstrass Institute for Applied Analysis and Stochastics
3: International School for Advanced Studies, Italy
4: University of Trento

14:00

We present a multiscale computational method for the efficient simulation of vascularized tissues. The work is motivated by the solution of inverse problems in the context of tissue imaging, where available medical data (such as those obtained via Magnetic Resonance Elastography) have a limited resolution, typically at the scale of an effective - macroscale - tissue, and cannot resolve the microscale of quantities of interests related, for instance, to the tissue vasculature.
Our model is based on a geometrical multiscale 3D (elastic) -1D (fluid) formulation handling the effect of a 1D fluid vasculature on a 3D elastic matrix with an immersed method.

At the solid-fluid boundary, we impose a trace-averaged boundary to model physically the normal inflation/deflation of the vessel wall.

The problem is solved using a Reduced Lagrange multipliers approach, which exploits the lower dimensionality of the fluid subdomain and allows for efficient numerical methods without requiring the discretization of the fluid-solid interface within the computational mesh.

Generation of organ-scale synthetic vasculature using mathematical optimization

Jessen, Etienne (1); Steinbach, Marc C. (2); Schillinger, Dominik (1)
1: TU Darmstadt
2: Leibniz University Hannover

14:20

The functional assessment of organs is essential for increasing the success of treatment strategies. Detailed information on the organ's vasculature could critically improve this assessment.

Extending our earlier work [1,2], we introduce a new framework to generate the complete vasculature of an organ synthetically. Our main contribution is the formulation of a nonlinear optimization problem (NLP) with super-linear time complexity. A second contribution is the addition of an extended problem, capturing the non-Newtonian behavior of blood. Lastly, we show how the problem of multiple, non-intersecting trees can be naturally included into the framework.

We compare our results against benchmarks for multiple anatomic regions of brain tissue and show that our framework outperforms current state-of-the-art algorithms [3] by an order of magnitude. Furthermore, we generate the complete liver vasculature with over five million vessels and compare them against measurements from the literature [4].

References

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A multi-compartment perfusion model of blood flow through deformed hierarchical vessel networks

Hohl, Jannes; Ebrahem, Adnan; Jessen, Etienne; Schillinger, Dominik
TU Darmstadt

14:40

For many physiological phenomena, such as tissue deformation or growth, an adequate perfusion model of the underlying hierarchical vascular network is of great interest. A fully resolved model on multiple spatial scales is still unattainable due to the mostly unknown complex structure of the vascular network. In order to obtain sufficiently accurate results with practical computational resources, a simpler perfusion model is required that still takes into account the hierarchically complex structure over different scales of the tissue and vessels [1]..

For this purpose, the vascular network is partitioned into a coupled multi-compartment model where the various hierarchies are represented by the compartments as continua with macroscopic laws [2]. The approach is to describe both the microscale and the hierarchies above as a porous medium using Darcy-type flow models that account for the different spatial scales. Based on synthetic vascular network model data essential parameters are determined for each compartment using averaging procedures. The interaction between the different compartments is considered via the pressure-dependent mass exchange and is applied in an averaged sense as well as the boundary conditions.

For the solution of deformation-dependent phenomena, iterative solution methods are usually required. Especially for parameters such as permeability, which depend on the geometry of the vascular network and thus on its deformation, the parameters would have to be determined anew in each iteration step. Since this is not in the interest of efficiency, a model for growth-induced deformations

was developed that simply updates the model parameters with deformation-dependent quantities only. This avoids the need for re-determination by averaging in each iteration step.

We illustrate an application to a liver growth model, where the microcirculation and the different hierarchies of the supplying and draining vascular trees are modeled as an independent compartment and the upper hierarchies not suitable for homogenization are considered as boundary conditions.

References

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Coupling of a perfusion model to a poroelastic-growth model for modeling liver tissue re-growth

Ebrahem, Adnan; Jessen, Etienne; Hohl, Jannes; Schillinger, Dominik 15:00
TU Darmstadt

Livers are able to regrow after injury. In practice, up to 75% of the liver can be removed during liver resections [1]. A liver resection is a common surgical procedure to remove part of the liver, mostly due to a tumor. Due to the multiscale nature of liver anatomy, the regrowth of the liver after resection is a process occurring over many scales which requires input and output values between different scales and is yet not fully understood. Currently no mechanistic mathematical model addresses liver regrowth after surgical resection.
Since the liver is characterized by a high degree of vascularization, blood perfusion and tissue re-growth are closely linked. Investigating the influence of perfusion on the mechanical behavior of the liver is of utmost importance due to possible application in surgical planning and surgery assessment. A detailed understanding of liver tissue mechanics in relation to perfusion significantly improves many clinical treatment strategies, including suitable cut patterns during liver resections [2].
In this talk, we present a framework for modeling liver tissue based on coupling a poroelastic-growth model with a fluid network to describe liver tissue deformation and blood flow. We present numerical examples, demonstrating the capability of the methodology to model liver tissue regrowth.

References

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Towards multi-scale model selection for rare data applications in life sciences

Reisch, Cordula (1); Nickel, Sandra (2); Tautenhahn, Hans-Michael (2) 15:20
1: TU Braunschweig
2: University Hospital Leipzig

Complex systems in life sciences often suffer from complicated or expensive data, leading to a lack of time- and space-dependent data.

Macro-scale models like reaction diffusion equations allow predictions of long-term behavior which can be associated with observations on a larger length scale. An example of those processes with rare data is liver inflammations. The dynamics leading to chronic inflammation are complex, and only the outcome of chronic inflammation is observable.

As the scales of mechanistic processes and observations vary widely, the reaction diffusion system is abstract, and a good representation of the mechanisms is not given a priori. One open challenge therefore is the connection of 1) the longtime behavior, 2) the abstract mechanisms in the reaction diffusion system, and 3) the known interactions on cell-scale.

We approach the challenges from two sides.

First, a model family of reaction diffusion equations is presented. Based on analytical properties like the longtime behavior of solutions, one model from the family is selected, [2].

Secondly, machine learning techniques are used for selecting models based on qualitative data like long-time observations. We present an algorithm for selecting mechanisms in an ordinary differential equation setting and show challenges that arise.

The combination of both approaches leads to a coupling of the different scales and takes advantage of all available information even in cases with little data.

References:

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Multiphase Modeling and Simulation of Function-Perfusion Processes in the Human Liver on Different Scales

Lambers, Lena; Gerhäusser, Steffen; Mandl, Luis; Ricken, Tim 15:40
University of Stuttgart

The liver has a complicated interaction between perfusion and functional activities on various length scales since it is a pivotal organ for essential metabolic functions.

This includes macroscopic perfusion in the total organ, microscopic perfusion in the functional units called liver lobules and function in the 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. [1,2], using a multicomponent mixture theory based on the Theory of Porous Media (TPM, see [3]).

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. The whole-body scale incorporates processes from other organs like kidney or lung.

We have developed a modular and efficient coupling to combine processes on the whole-body, lobule and cell scale using a coupling library resulting in a tri-scale PDE-ODE approach. This approach allows the simulation of processes like detoxification, zonated fat accumulation or ischemia-reperfusion injury during transplantation.

As a first step to improve the model for clinical usability, hybrid knowledge- and data-driven approaches have been developed using experimental, clinical and in silico data from cooperation partners [4]. Here, histological sections provide realistic geometries of the liver lobules, that serve as input geometries for the simulations. Furthermore, the inclusion of patient-data provided from clinical cooperation partners enable an individual simulation of hepatic processes.

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S02.08: Mechanobiology

Date: March 22, 2024 08:30–10:30
Room: G22/111
Chair(s): Abdolazizi, Kian

Enhancing Leg Alignment in Adolescents: Exploring Optimal Positioning of Tension Band Implants for Guided Growth - A Finite Element Investigation

Hucke, Lucie (1,2); Vincenti, Sonia (1,3); Holder, Jana (4,5); van Drongelen, Stefan (6); Braun, Sebastian (4,7); Schwer, Jonas (8); Seitz, Andreas (8); Stief, Felix (4,6); Huß, Armin (1); Gámez, Antonio (2); Wittek, Andreas (1)

1: Frankfurt University of Applied Sciences
2: University of Cádiz, Spain
3: Offenburg University of Applied Sciences
4: University Hospital Frankfurt, Goethe University Frankfurt
5: Current affiliation: University of Salzburg
6: Dr. Rolf M. Schwiete Research Unit for Osteoarthritis, University Hospital Frankfurt, Goethe University Frankfurt
7: Current affiliation: Charité – Universitätsmedizin Berlin, corporate member of FU Berlin and Humboldt-Universität zu Berlin, Center for Musculoskeletal Surgery
8: Ulm University Medical Centre

08:30

Indroduction: Positioning of the tension band implant is essential and variable in guided growth [1], directly affecting treatment outcomes. It alters stress distribution in the growth plate (GP) and thus influences growth in the blocked joint [2]. A previous study [3] investigated the influence of the implant on stress distribution using a personalized finite element (FE) simulation for three patients; however, the model was not validated and the influence of different implant positions was not analyzed. To address this limitation, this study evaluated the GP stress distribution using a validated FE model and various tension band implant positions.

Methods: For the purpose of model validation, six porcine knees underwent loads up to twice their body weight, with GP deformation measured by MRI [4]. Using the MRI images of the unloaded knee, an FE model was created and simulated under known boundary conditions from the test setup. To analyze the positioning parameters, the surgical data from guided growth treatments of 34 patients with malalignment were evaluated [1], and the minima and maxima of each parameter were determined and applied to the validated FE model. The stress distributions resulting from these implant positions were compared to those observed when the implant was positioned according to the manufacturer's recommendations.

Results: The initial findings of the FE simulation revealed that stress within the entire GP, not just on the implant side, was influenced by different implant and screw positions. The study's findings identified the positioning parameters that have a significant influence on the stress in the GP.

Conclusion: This study was conducted with identical geometry to isolate the influence of positioning parameters from the influence of geometry; it may help to better understand the influence of implant positioning.

References:

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[4] Schwer (2020); Front. Bioeng. Biotechnol.; 8

Application of the Neighbored Element Method on a Hamilton principle-based multi-species biofilm model

Klempt, Felix; Soleimani, Meisam; Junker, Philipp

Leibniz University Hannover

08:50

In order to help patients suffering from teeth loss, oral implants have proven themselves to be a viable and highly successful long term solution. However, since the oral microbiome consists of several hundreds of species of microorganisms and thus is one of the most complex microbial communities, it comes to no surprise that the introduction of man-made implants can lead up to infectious diseases in the oral cavity. For example, peri-implantitis, an infection of the gum and bones, is caused by communities of the oral microorganisms with serious consequences for the patients such as a

reduction of bones and consequently implant failure. These communities are called "biofilm" and attach themselves to the implant surface. In an effort to reduce cases of biofilm induced implant failure, it is crucial to understand the innerworkings of biofilms. Hereby, *in silico* experiments are a vital tool to complement *in vitro* and *vivo* experiments. When performing *in silico* experiments, a sensible material model is crucial. In literature, current biofilm growth models either follow a volumetric or a density based approach. In the volumetric approach, the deformation gradient is split into an elastic and a growth part, similar to plastic strain models. In the density based approach, the density evolves according to an evolution equation. In neither model, the consistency with the second law of thermodynamics is usually checked, but instead they are phenomenologically motivated. Biological systems are treated in the context of an open system, in which one assumes that energy, mass and entropy can be exchanged through the boundaries. This assumption poses serious challenges to thermodynamic consistency conditions. The model presented in this work is derived by an extension of the Hamilton principle and thus fulfills the thermodynamic consistency conditions automatically. In addition, both approaches mentioned earlier are combined to give a more general picture on growth behavior of biofilms. To capture the complexity of biofilm in the oral cavity, the model is extended to incorporate more than one type of biofilm. Both types of biofilm can grow independently and can either inhibit or promote each other's growth. The integration of multiple types of biofilm requires a lot of computational effort. The model is thus solved by using the Neighbored Element Method, a combination of the Finite Element Method and Finite Difference Method.

Cell-preserving Scheme for Mechanobiological Research on Dedifferentiation of Chondrocytes

Lee, Hyun; Tandale, Saurabh; Topol, Heiko; Stoffel, Marcus 09:10
RWTH Aachen University

In the present work, we introduce a scheme for efficient mechanobiological research on the dedifferentiation of chondrocytes using a deep neural network model that does not require sacrificing the cells and thus, saving resources. Cells are a part of active biological systems subjected to physical stimuli such as mechanical loading. Such loading affects cellular processes including proliferation, differentiation, and the interplay with the surrounding environment **[1, 2]**. Chondrocytes are mechanosensitive cells that produce and maintain the cartilaginous matrix that allows cartilage to bear and distribute mechanical loads in joints **[3]**; their role in cartilage regeneration and treatment of osteoarthritis (OA) has been the focus of research projects **[4]**. Nevertheless, it remains an open challenge to fully understand the effect of mechanical stimuli on chondrocytes **[5]**. One of the unresolved mechanobiological behaviors of chondrocytes is dedifferentiation. Dedifferentiation of chondrocytes is the phenomenon where isolated chondrocytes alter their phenotype when cultured in a 2D *in vitro* environment over passages **[6].** While intact, cobblestone-shaped chondrocytes mainly produce collagen II, dedifferentiated chondrocytes with elongated shapes produce fibroblastic collagen I **[7]**. This limits the scalability of a promising treatment for OA, called 'autologous chondrocyte implantation'. To overcome this limit, research is being undertaken to find the mechanism of dedifferentiation **[8]**.

This proposed scheme is composed of three parts: (i) the cell-seeded specimens are loaded in a bioreactor system **[9]**, (ii) an optical microscope is used to obtain the phase-contrast images of living cells, and (iii) the images are analyzed using a deep neural network **[10]**. This scheme provides an efficient tool to analyze the ratio of intact to dedifferentiated chondrocytes while preserving cells on our way to elucidate the effects of mechanical loading on the dedifferentiation of chondrocytes.

References:

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A refined model for the coupled analysis of actice biological processes for meniscus tissue regeneration

Jäger, Henry Sebastian (1); Grosjean, Elise (2); Simeon, Bernd (1); Surulescu, Christina (1)
1: RPTU Kaiserslautern-Landau
2: INRIA, France

09:30

Meniscus tears are one of the most frequently occuring injuries which people incur doing contact sports. They can cause severe chronic knee pain, stiffness and immobility which can potentionally end in a total knee replacement. Over the last decades, a trend arose to rather heal by regeneration and repair than to replace the damaged issue. On the other hand, mathematical modeling and numerical simulation of medical and biological processes have become an important tool for developing new methods for regeneration. They may allow to extend study results to related mutually processes. Although meniscus tissue engineering has recently attracted much interest, mathematical models and numerical simulations for the specific dynamics of the involved phenomena are still relatively scarce. In this presentation, we report about ongoing work on in silico research for the better understanding of an experimental study for meniscus regeneration. In essence, this experiment uses a nonwoven scaffold that is colonized by chondrocytes and adipose tissue-derived stem cells. The mathematical description involves active processes at the cell level, such as cell differentiation and matrix synthesis, that have a strong impact on the resulting tissue structure and quality, while macroscopic effects in turn are important stimuli for the processes at the microscopic level. The corresponding mathematical model consists of a set of coupled nonlinear parabolic partial differential equations where further effects, such as the flow of nutrients through the porous media of the scaffold and the mechanical deformation, can also be taken into account. From the numerical point of view, not only the forward simulation with vastly differing time scales but also the computation of parameter sensitivities represent a big challenge.

The presentation concentrates in particular on the numerical treatment based on a spatial discretization by a discontinuous Galerkin approach where also the orientation of the fibre structure in the scaffold is considered. We analyze the influence of the boundary conditions and the initial data, demonstrate the outcome of the in silico experiment for different scenarios and assess the possible feedback for the in vitro experiment.

S03: Damage and fracture mechanics

Organizer(s): Ricoeur, Andreas *(Universität Kassel)*
Gerke, Steffen *(Universität der Bundeswehr München)*

S03.01: Damage and fracture mechanics 1

Date: March 19, 2024 08:30–10:30
Room: G22/013
Chair(s): Brepols, Tim

A comparison of micromorphic gradient-extensions for anisotropic damage

van der Velden, Tim; Brepols, Tim; Reese, Stefanie; Holthusen, Hagen 08:30
RWTH Aachen University

The modeling of inelastic phenomena with tensor-valued internal variables requires a regularization to counteract mesh dependence. Here, we consider the regularization of anisotropic damage at finite strains and seek for an efficient formulation based on a reduced number of nonlocal degrees of freedom. We, thus, equip the brittle version of [1] with three different gradient-extensions in the micromorphic framework of [2] using one full and two reduced regularizations of the damage tensor. The models are investigated in structural simulations and compared with respect to their structural responses and the resulting failure patterns. High agreement is observed between the full regularization with six nonlocal degrees of freedom and a reduced volumetric-deviatoric regularization with two nonlocal degrees of freedom.

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Model order reduction for problems involving gradient-extended damage and plasticity

Brepols, Tim; Kehls, Jannick; Kastian, Steffen; Reese, Stefanie 08:50
RWTH Aachen University

The modeling and simulation of damage and fracture processes in materials is an important topic in mechanics, as it can help to improve the safety and durability of structures in a variety of engineering applications. Unfortunately, in practice, such simulations can be computationally very expensive. One way to counteract the computational effort is to apply model order reduction (MOR) techniques, which typically aim to reduce the global degrees of freedom of a discretized model system while keeping the introduced approximation error as small as possible.

A well-known representative of this class of methods is the proper orthogonal decomposition (POD), which belongs to projection-based MOR approaches. The basic idea is to project large systems into lower dimensional subspaces by extracting only their dominant modes and constructing appropriate projection matrices. For linear problems, this strategy works rather well. In countless cases, POD has proven its ability to tremendously reduce the number of unknowns and, thus, the computational complexity. For nonlinear problems, however, the situation becomes much more complicated, since the dominant modes are subject to change and the projection matrices themselves need to be updated, partially diminishing the speedup potential of the method. For this reason, hyperreduction techniques such as the discrete empirical interpolation Method (DEIM) have been developed, essentially providing a second layer of reduction that helps to overcome the shortcomings of POD in nonlinear problems [1]. DEIM has already been successfully applied in hyperelastic and viscoelastic structural problems, see e.g. [2].

The present study is concerned with the development and investigation of a novel POD+DEIM-based approach to accelerate finite element simulations making use of a highly nonlinear gradient-extended

damage-plasticity material model for describing fracture phenomena in (quasi-)brittle and ductile materials [3]. In this context, a reduced arc-length method is proposed, which allows the calculation of softening problems where snapback behavior occurs. Furthermore, the novel idea of constructing separate projection matrices for the physically very different nodal degrees of freedom (displacements and nonlocal damage) is investigated in detail.

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A gradient-extended two-surface damage-plasticity model based on the star-convex decomposition of the strain energy

Zhang, Jian; Brepols, Tim; Reese, Stefanie
RWTH Aachen University

09:10

The gradient-extended two-surface damage-plasticity model reported by Brepols et al. [1,2] has great flexibility in dealing with the failure process between brittle material and ductile material. This is because damage and plasticity are considered distinct but strongly coupled physical mechanisms by using separated damage and plastic yielding criteria and related loading/unloading conditions [1,2]. However, there are three evident drawbacks in the standard gradient-extended two-surface damage-plasticity model. Firstly, the tensile and compressive strengths at the onset of damage have the same magnitude which is unrealistic for most materials. Secondly, for the given material parameter, once the tensile strength is determined, there is no flexibility to match the experimentally known values of the compressive and shear strengths. Finally, the standard model cannot model the unilateral contact under compressive loading when the material is fully broken. To solve the mentioned shortages of the standard model, the star-convex decomposition of the total strain energy proposed by Vicentini et al. [3] is adopted in the current model. In the end, a numerical example is provided to show the properties of the present model in simulation.

Theoretical and Applied Strategies for Numerical Damage Optimisation

Guhr, Fabian; Barthold, Franz-Joseph
TU Dortmund University

09:30

Accurate modelling in metal forming is a complicated but important step for precise predictions of material behaviour under operational loads or during the forming process. While modelling of plasticity effects is a well-established field, ductile damage is nowadays also important to consider in simulations. Theoretically, damage mechanics should not be critical for a final product under operative loads. Its consideration for forming simulations, however, is very important to predict the damage state and hence the performance of a produced part. With accurate damage models, it is furthermore possible to enhance a product by applying numerical optimisation.

Numerical damage optimisation can be applied in multiple ways and environments. For gradient-based optimisation, the gradients with respect to the design variables of the optimisation problem are required. When applying sensitivity analysis to regularised, non-local damage models, the additional global damage variables and their additional global equilibrium equations have to be handled accordingly [1]. Furthermore, the addition of state-dependent history variables, introduced with plasticity and local damage modelling, must be taken into account when deriving the gradients. This in turn leads to additional requirements for the numerical implementation, i.e. a history sensitivity update after each load-step. When implemented correctly, analytical gradients are very efficient. In forming however, contact mechanics is a key component. Derivation of analytical gradients of such a discontinuous problem is very complex. It can be circumvented by utilising commercial FEM software, which runs the simulations and handles contact mechanics. This allows creation of a framework which enables optimisation with the software solely as the FEM solver [2].

This talk gives an overview of applied numerical optimisation from two different viewpoints. By enhancing a non-local damage model with sensitivity analysis, it is possible to generate damage tolerant parts which show less damage accumulation. Additionally, the benefit of utilising a damage

model in numerical optimisation is highlighted. In contrast to the analytical approach, a framework is presented which enables optimisation of existing forming simulations within Abaqus. Numerical optimisation is applied to forming processes to enhance their capabilities with respect to damage accumulation and optimal process parameter sets are generated

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An implicit gradient-enhanced microplane damage material model in the coupled implicit MPM-FEM

Oropeza Navarro, Osvaldo Andres; Chihadeh, Ahmad; Platen, Jakob; Kaliske, Michael 09:50
TU Dresden

The Material Point Method (MPM) attracts an increasing interest due to its capability to model problems involving large deformations. However, MPM comes with a larger computational cost compared to the Finite Element Method (FEM). Consequently, to achieve computational efficiency, formulations that combine MPM and FEM have emerged. As of the authors' knowledge, these approaches have successfully addressed a monolithic coupling between MPM and FEM, but fail when the material description is based on nonlocal mechanics. Moreover, complex material models require often a nonlocal formulation to overcome problems of numerical instabilities, that can arise when modelling strain softening behavior

In this work, a new approach for monolithic MPM-FEM coupling including a nonlocal formulation is developed. The coupling between both discretization methods is addressed by bond elements. A novel formulation of nonlocal bond elements is introduced in this work, which couples the mechanical and nonlocal fields between both discretizations in an effective manner.

Furthermore, a constitutive law at finite deformations to describe fiber reinforced concrete is applied. A damage formulation within the microplane framework is utilized to capture the induced anisotropy in concrete structures. Furthermore, the microplane model is able to capture the initial anisotropy due to fiber inclusion. Moreover, implicit gradient-enhancement is utilized to regularize strain localization problems. Finally, numerical examples are focused on showing the potential of bond elements to effectively transmit nonlocal fields regardless of the orientation or discretization, model finite deformation and reproduce experimental results within the coupled MPM-FEM.

S03.02: Damage and fracture mechanics 2

Date: March 19, 2024 16:30–18:30
Room: G22/013
Chair(s): Kozinov, Sergey

Fracture modeling of flexoelectric materials with mixed FE

Serrao, Prince Henry; Kozinov, Sergey 16:30
Ruhr University Bochum

Direct flexoelectricity is the higher-order, two-way electromechanical coupling between strain gradients and the electric field. Due to its inherent size effects, it is very prominent at smaller scales, with profound applications to high-precision micro- and nano-electromechanical systems such as sensors, actuators, energy harvesters, etc. Flexoelectricity in linear dielectrics [1] and piezoelectrics [2] has been recently analyzed in detail. However, the fracture behavior of flexoelectric solids is still not explored, though in the vicinity of the crack tips there are naturally occurring strain gradients. In the current work, the robust mixed FE proposed in [2] is extended for the fracture mechanics calculations. The analysis of the crack tip opening displacements (CTOD) and the variations of electric potential along the crack front has been done. In addition, a post-processing script is developed

to trace the evolution of the configurational forces and their spatial distribution. The configurational forces represent the thermodynamic driving forces acting on the defect [3], while the J-integral can be easily evaluated using the configurational force at the crack tip. Using these computations, the influence of strain gradients and flexoelectricity is investigated. Further, the influence of the flexoelectric coefficients and the direction of the ceramic polarization are examined. Current work explores the interplay of the linear and the higher-order electromechanical coupling, described by piezoelectricity and flexoelectricity, in the presence of the crack in the realm of linear elastic fracture mechanics.

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[3] Kozinov, S., Kuna, M., 2023. *Configurational forces in ferroelectric structures analyzed by a macromechanical switching model*. Acta Mech 234, 17–36.

Multiscale damage analysis based on the variational effective model

Xu, Xu (1); Jezdan, Ghina (2); He, Yiqian (1,2); Hackl, Klaus (2)
1: Dalian University of Technology, China
2: Ruhr University Bochum

16:50

In the damage analysis of material with complex microstructures, a full-scale direct numerical simulation (DNS) could produce huge computational costs. Alternatively, the multi-scale modeling is a more effective method by using less degrees of freedom to balance the calculation accuracy and cost. In this paper, a new multiscale damage modeling method is proposed based on the variational effective model originally presented by Jezdan et al. and the relaxation damage model presented by Junker et al.. A variational statement for the free energy and the dissipation potential for a coarse scale model is constructed by relating the free energy and dissipation potential of the fine scale model. In this way, the coarse scale damage variable is defined instead of directly solving in the fine scale model, therefore the computational efficiency can be increased. Besides, the relaxation damage model can effectively avoid ill-posed boundary value problems in damage analysis without use of gradients or complex integration techniques. Finally, we provide three numerical examples to demonstrate the accuracy and efficiency of the proposed method.

A finite element framework for thermo-mechanically coupled gradient-enhanced damage formulations

Sobisch, Lennart (1); Kaiser, Tobias (1); Menzel, Andreas (1,2)
1: TU Dortmund University
2: Lund University

17:10

The characterisation of damage and degradation mechanisms constitutes a major part in modelling industrial processes such as metal forming. A common regularisation strategy for damage models is obtained by the incorporation of additional gradient contributions into the constitutive equations. In a thermo-mechanically coupled setting, gradient-enhanced damage models result in a problem of three coupled field equations. The solution of multi-field problems and the numerical implementation by means of the finite element method constitute a sophisticated part of the characterisation of complex material behaviour. Particularly the implementation into commercial finite element codes is of importance for practical and industrial applications. An Abaqus UMAT framework was introduced in [1, 2] for the implementation of arbitrary two-field problems. An extension of the framework to the solution of three coupled field equations (and potentially more) is presented in this contribution.

A comprehensive implementation framework for micromorphic continua in a thermo-mechanically coupled setting into the finite element software Abaqus is provided. The framework is exemplarily applied to a gradient-enhanced damage model. Representative simulation results are discussed on a local and a global level to assess the implementation framework and the extension to arbitrary multi-field problems is discussed.

Neural networks meet phase-field: A hybrid fracture model for elastomers

Dammaß, Franz; Kalina, Karl; Kästner, Markus 17:30
TU Dresden

For the mechanical behaviour of elastomers, micromechanically-informed constitutive models that are based on statistical mechanics have proven of high value, for instance the*non-affine unit sphere model* [1]. However, these approaches are computationally expensive, since chain statistics have to be evaluated for a representative set of microscopic chain directions for each macroscopic material point. Likewise, for the prediction of fracture, the phase-field approach has become a well-established tool, although it comes along with a severe computational effort since it requires small time steps and fine meshes.

Physics-augmented neural networks (NNs) become increasingly popular for constitutive modelling, and have shown to be suitable surrogates for hyperelastic materials, see e.g. [2]. Apart from their flexibility for describing complex experimentally-observed material responses, these approaches may also reduce computational effort compared to classical micromechanically-informed models.

This contribution aims at combining the predictive capability of the phase-field approach to fracture with the advantages of NNs by means of a *hybrid* model of fracture. To this end, conceptionally, a pseudo-energy functional is introduced, cf. [3], that combines a hyperelastic neural network-based free energy potential, and the classical phase-field fracture dissipation potential.

[1] C. Miehe *et al.*, 'A micro-macro approach to rubber-like materials—Part I: the non-affine micro-sphere model of rubber elasticity', *Journal of the Mechanics and Physics of Solids*, Nov. 2004.

[2] L. Linden *et al.*, 'Neural networks meet hyperelasticity: A guide to enforcing physics', *Journal of the Mechanics and Physics of Solids*, Oct. 2023.

[3] F. Dammaß *et al.*, 'The rate- and temperature-dependent ductile-to-brittle fracture transition of toffee-like caramel: Experimental investigation and phase-field analysis', *arXiv preprint*, Nov. 2023.

A multi-field decomposed model order reduction approach for thermo-mechanically coupled multiphysics simulations including damage

Zhang, Qinghua 17:50
RWTH Aachen University

Predicting and analyzing damage initiation and propagation in ductile materials under thermomechanical scenarios has significant implications for research and industry. Many models in the literature concentrate solely on fracture and damage mechanisms, neglecting the influence of temperature. As a result, simulations based on such models are often only adequate for a few special cases that are far away from the actual manufacturing conditions. Therefore, the integration of efficient model order reduction techniques into multiphysics models is an interesting and promising area of research, especially for industries focusing on real-time simulations.

The primary objective of this work is to combine the model order reduction technique with the gradient-extended damage-plasticity formulation for finite strains by Brepols et al. [1] and to study its effect on reducing computational costs. Then, a multi-field decomposed POD is integrated into the thermo-mechanically extended version of the aforementioned model (see Felder et al. [2]) to enable fast multiphysics damage-plasticity simulations. Finally, the new approach is investigated in several numerical benchmark tests to evaluate its advantages and disadvantages.

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A novel approach for a thermo-mechanically coupled and gradient-enhanced damage model
Liu, Fangrui; Jantos, Dustin Roman; Junker, Philipp
Leibniz University Hannover
18:10

Material damage leads to an increase in temperature due to energy dissipation. Furthermore, a non-uniform temperature distribution can result in damage evolution due to the internal stress in a physical body. To model this behavior, we apply the extended Hamilton's principle to create a new thermo-mechanically coupled gradient-enhanced damage model, which includesthe damage and temperature evolution. In order to accelerate the computation speed, we adopt the neighbored element method to calculate the Laplace operator for the damage variable and temperature in the governing equation. The numerical examples show the robustness and efficiency of our method in the thermal shock problem.

S03.03: Damage and fracture mechanics 3

Date: March 20, 2024 14:00–16:00
Room: G22/013
Chair(s): Gerke, Steffen

Microscale Modeling of Damage Mechanisms in Dual-Phase Steel DP800
Niehüser, Alexander; Mosler, Jörn
TU Dortmund University
14:00

Dual-phase steels are very popular in the automotive industry due to their high strength while maintaining good formability. The macroscopic formability of this polycrystalline material is governed by deformation and damage mechanisms at the microscale. To describe the mechanical properties associated with these mechanisms, a crystal plasticity theory is coupled with interface models and integrated into (statistical) representative volume elements (RVEs). The interface models capture decohesion at the grain boundaries as well as the initiation and propagation of micro-cracks (damage) within the quasi-brittle martensite phase of the dual phase steel DP800. In this contribution, the focus lies on the numerically efficient implementation of the these models by means of the finite element method. The interaction and activation of the different (damage) mechanisms will be investigated.

INFLUENCE OF IMPACT LOADING ON CREEP, DAMAGE AND FRACTURE OF METALS
Breslavsky, Dmytro (1,2); Tatarinova, Oksana (1); Altenbach, Holm (2)
1: National Technical University "Kharkiv Polytechnic Institute", Ukraine
2: Otto von Guericke University Magdeburg
14:20

Many structural elements of modern aerospace and power industrial components work at high temperatures. Under these conditions, creep strains develop in their material, and as a result of creep, damage accumulation develops, which lead to fracture process arising. On the other hand, in the process of operation, it is possible to receive one or a series of impacts on the surface of the structural element. Such additional loads, for example, occur in the blades of gas turbines with repeated contact with the surface of the housing. Even in the absence of instantaneous failure, impact loads of low intensity can affect the processes of deformation and damage accumulation and intensify them.

A general boundary - initial value problem is formulated for the description of creep- damage processes. For the case of impact cycles, the formulation of the problem using the methods of many time scales and period averaging is considered.

Attention is paid to the formulation of constitutive and evolution equations. Materials whose creep damage can be described using evolution equations with a scalar (steel) or tensor damage parameter (light alloys) are considered. The influence of a single impact load on the stress-strain state during creep is taken into account in the creep rate equation for the description of overloads. In the case of repeated, cyclic impact contacts, the method of many time scales and period averaging is used. As a method of solving the boundary-initial value problem, the Finite Element Method was used in combination with the method of time integration. After determining the completion of hidden

failure in a certain finite element, the process of further fracture development is considered. For this purpose, an algorithm for removing elements from the model with a complete reformulation of the boundary - initial value problem with new boundary conditions is used. The initial conditions are determined by the current distributions of stresses, strains, displacements and damage parameter.

The processes of creep-damage and fracture are considered for the case of a plane stress state. The results of modeling creep-damage processes that develop after impact loading in steel and titanium alloy plates are presented. The distributions of creep strains and damage are considered. The deformed state in the steel plate under the conditions of its fracture development due to the accumulation of creep damage was analyzed.

Concurrent Approximation of Rank-One Convex Envelopes with Application to Continuum Damage Mechanics

Köhler, Maximilian (1); Neumeier, Timo (2); Peter, Malte A. (2); Peterseim, Daniel (2); Balzani, Daniel (1)
1: Ruhr University Bochum
2: University of Augsburg

14:40

Relaxation techniques, particularly in the context of finite element simulations, offer a powerful means to incorporate complex microstructures without introducing additional length scale parameters. However, integrating concurrent numerical relaxation for rank-one convexification within incremental, dissipative models often imposes considerable computational overhead, see [1], limiting its practical application. This presentation introduces a novel algorithm leveraging hierarchical sequences (H-sequences, see [2, Definition 5.14]) to approximate and establish an upper bound for the rank-one convex envelope. Notably, this method aligns with the rank-one convex envelope for materials achieving energetic optimality at each laminar level. Demonstrating applications in non-convex finite strain continuum damage models (cf. [3] for the recapitulated derivation), particularly in two and three dimensions, this approach facilitates concurrent numerical relaxation within large strain models, ensuring compatibility of the implied microstructure. The talk explores various aspects of the algorithm, including restoring rotational invariance, microstructure reconstruction, comparative analysis with other semi-convex envelopes, derivative information, and considerations regarding mesh dependency.

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On the path-dependence of ductile damage models

Feike, Klas; Langenfeld, Kai; Kurzeja, Patrick; Mosler, Jörn
TU Dortmund University

15:00

Ductile damage - damage associated with plastic deformation - leads to a degradation of material properties and is an important aspect in many technical applications, e.g. in metal forming processes, cf. [1]. Although such a degradation cannot be completely prevented, it is undesirable and must therefore be controlled. To understand degradation - both qualitatively and quantitatively - continuum damage theory provides a natural framework. Very often the corresponding models depend on stress invariants, e.g. triaxiality and Lode angle. Although such an assumption is intuitive, it often represents a relatively crude simplification, see [3,4]. Especially when complex load paths and anisotropic effects become important, further influences of the stress state have to be considered.

In this work, the (anisotropic) damage evolution is carefully analyzed using two established models suitable for ductile damage evolution, c.f. [5,6]. Different loading paths are chosen to (i) show the limitations of the simplified approach and (ii) derive new indicators for damage initiation and evolution. On the basis of these new indicators, optimized stress paths are derived that show less damage.

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[2] Langenfeld, K. and Mosler, J. (2019). A micromorphic approach for gradient-enhanced anisotropic ductile damage. Computer Methods in Applied Mechanics and Engineering 360. 112717.

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Mixed finite element implementation of plane crack problems within strain gradient elasticity

Chirkov, Aleksandr Yu. (1); Nazarenko, Lidiia (2); Altenbach, Holm (2)

1: Pisarenko Institute of Problems of Strength, NAS of Ukraine
2: Otto von Guericke University Magdeburg

15:20

An alternative approach is proposed and applied to solve boundary value problems within the strain gradient elasticity theory. A mixed variation formulation of the finite element method (FEM) concerning displacement-strain-stress is used, adopting the governing equations for stresses, strains, and displacements as independent variables. This significantly simplifies the pre-requirement for approximating functions to belong to class C^1 and allows one to use the simplest triangular finite elements with a linear approximation of displacements under uniform or near-uniform triangulation conditions. Global unknowns in a discrete problem are nodal displacements, while the strains and stresses in nodes are treated as local unknowns. The conditions of existence, uniqueness, and continuous dependence of the solution on the problem's initial data are formulated for discrete equations of mixed FEM. These are solved by a modified iteration procedure, where the global stiffness matrix for classical elasticity problems is treated as a preconditioning matrix with fictitious elastic moduli. This avoids the need to form a global stiffness matrix for the problem of strain gradient elasticity since it is enough to calculate only the residual vector in the current approximation. A set of modeling plane crack problems is solved. The obtained solutions agree with the results available in the relevant literature. Good convergence is achieved by refining the mesh (finite element length) for all scale parameters. All three problems under study exhibit specific qualitative features characterizing strain gradient solutions, namely crack stiffness increase with length scale parameter and cusp-like closure effect.

Analysis of failure of fibre-reinforced high performance concretes due to low cycle fatigue

Pise, Mangesh (1); Brands, Dominik (1); Gebuhr, Gregor (2); Anders, Steffen (2); Schröder, Jörg (1)

1: University of Duisburg-Essen
2: University of Wuppertal

15:40

In recent decades, extensive research has led to the development of more efficient and stronger types of concrete, including high performance concrete (HPC) and ultra high performance concrete (UHPC). These materials are becoming increasingly popular in the global construction industry. Steel fibres, especially hookedend fibres, are commonly added to enhance the ductility of HPC, whereas short, straight fibres are usually added to UHPC. The fibre reinforcements increase ductility by transmitting stresses from the matrix to the fibres during fracture. This process shows pronounced effect on the

deterioration characteristics of concrete in cyclic flexural tests, see [2].
The purpose of this contribution is to examine how the orientation and distribution of fibres affect the overall material behaviour of fibre-reinforced HPCs and UHPCs during low cyclic fatigue. A phenomenological material model has been developed by combining the superposed models of transversely isotropic elasto-plasticity, see [1], and a continuum phase-field model of fracture in elasto-plastic material, see [3, 4]. Two continuous stepwise linear degradation functions are used to model the unsymmetric behaviour of (U)HPC in tension and compression. The numerical model is calibrated using experimental data and simulating typical uniaxial cyclic tests and three-point bending beam tests at low cycle for pure (U)HPC. Low cycle three-point bending beam tests are simulated for reinforced (U)HPCs with different fibre contents and orientations. To account for the different distributions and orientations of the fibres, 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].

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S03.04: Damage and fracture mechanics 4

Date: March 20, 2024 16:30–18:30
Room: G22/013
Chair(s): Kiefer, Bjoern

M-Integral and energy-release rates: A didactical account

Kienzler, Reinhold (1); Nguyen, Anh Tay (2); Pak, Y. Eugene (3) 16:30
1: University of Bremen
2: Northwestern University,USA
3: SUNY Korea

Within the framework of linear elasticity, the M-integral is connected to energy changes due to a self-similar expansion of a configuration. In this contribution, we will calculate the M-integral by evaluating a path-independent contour integral and by calculating the virial of material tractions active at boundaries and interfaces for the simple case of a hollow circular cylinder having an inclusion with and without misfit, loaded by external forces under plane stress/plane strain conditions. The connection between the similarity transformation of the total elastic potential and the M-integral is explored.

Lifetime prediction for cyclic material behavior – Application to multiaxial fatigue

Langenfeld, Kai (1); Desmorat, Rodrigue (2); Kurzeja, Patrick (1); Mosler, Jörn (1) 17:30
1: TU Dortmund University
2: ENS Paris-Saclay, France

Predicting failure due to fatigue remains a fundamental challenge in the field of 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 induce decohesions and cracks nucleation at the micro level, which subsequently coalesce into macro cracks, cf. [1]. Numerous models are available in the

literature in order to predict the initiation of damage at the macro level. Critical plane approaches, for example, prove to be efficient tools for the prediction of the lifetime of components and structures under 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.

A first damage initiation criterion in the spirit of continuum damage mechanics is based on the stored energy function [1]. This criterion has been extended to additionally account for the plastic strain amplitude in [3] to easily distinguish between different load amplitudes on the local level.

Within this talk, a new damage initiation criterion will be formulated to account for multiaxial fatigue. First, a damage model suitable for ductile material degradation will be extended to account for the different mechanisms associated with cyclic tension and cyclic torsion. Subsequently, the damage initiation criterion in [3] will be modified. To be more precise, the inclusion of the Lode angle allows to explicitly account for the degree of multiaxiality. The capabilities of the extended criterion will be demonstrated by means of fatigue experiments. It will be shown that this extension is necessary to capture both failure associated with tension and failure associated with torsion in a unified approach.

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Geometric and Constitutive Modeling of MgO-C Refractories Based on Recyclates for Thermo-Mechanical Simulations

Gopi, Jishnu Vinayak; Roth, Stephan; Kiefer, Bjoern 17:50
TU Bergakademie Freiberg

Refractories are polycrystalline, porous, heterogeneous, non-metallic materials utilized as protective liners in high-temperature manufacturing processes. Microscopic and mechanical characterization studies of MgO-C refractories in the literature show a strong correlation between the underlying microstructure and the thermo-mechanical response of these materials. The present study focuses on developing a simulation tool that evaluates the thermo-mechanical behavior of recycled refractories, specifically the influence of microstructural features on their thermal shock resistance. In contrast to prior methodologies [1,2], the intricate and heterogeneous microstructure of MgO-C is conceptualized as a three-phase composite comprising coarse magnesia aggregates, graphite flakes, and an effective matrix. The homogenized matrix material is presumed to consist of fine magnesia, carbonaceous binders, additives, and pores. A pre-processing tool with a graphical user interface (GUI) is developed to synthetically generate this idealized 2D microstructure representation from statistical data, such as particle size distributions and phase volume fractions, utilizing open-access Python packages [3]. According to the current hypothesis and experimental findings, the principal mechanism of damage in these materials involves the debonding of phase interfaces due to thermally induced stresses. This interface damage is modeled using the cohesive zone approach. Basic thermal shock simulations are performed employing the synthetically generated microstructure to investigate the influences of thermal expansion coefficient mismatches and thermal gradients on the local interface damage as well as the initiation and propagation of macroscopic cracks. Furthermore, a sensitivity study is presented to analyze the influence of particle size distribution on the thermal shock resistance of these refractory composite materials.

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Analysis of damage and failure behavior of additively manufactured stainless steel 316L by biaxial experiments

Gerke, Steffen (1); Diller, Johannes (2); Pérez Cruz, Leonardo Daniel (1,3); Blankenhagen, Jakob (2); Mensinger, Martin (2); Brünig, Michael (1)

1: University of the Bundeswehr Munich
2: Technical University Munich
3: Universidad Nacional de Mar del Plata, Argentina

18:10

The austenitic stainless steel AISI 316L (1.4404) is frequently used in medical applications as well as in aerospace and automotive industries due to its corrosion resistance and high ductility. Individual parts and smaller series as well as more complex geometries can be produced by powder bed fusion of metals using a laser (PBF-LB/M), i.e. additive manufacturing. The components produced in this process not only have different mechanical properties compared to components made from conventionally produced base material by cutting machining processes. Also, the multiaxial stress state behavior of PBF-LB/M/316L has not been investigated yet

The presentation deals with an initial experimental series with additively manufactured biaxial specimens made of AISI 316L stainless steel. The biaxial specimen geometry has been specially adapted for the requirements of PBF-LB/M and the specimens are loaded under different biaxial proportional load paths up to failure. Accompanying numerical simulations are performed to determine the associated stress state and analyze the existing stress-dependent damage and failure mechanisms. The formation of strain fields in critical parts of the modified H-specimen is monitored by digital image correlation at various points of the experiment and the different failure modes are visualized by scanning electron microscopy of the fracture surfaces.

S03.05: Damage and fracture mechanics 5

Date: March 21, 2024 08:30–10:30
Room: G22/013
Chair(s): Löhnert, Stefan

A monolithic approach to the phase-field modeling of brittle fracture using the scaled boundary finite element method

Pasupuleti, Ajay Kumar (1); Assaf, Rama (1); Birk, Carolin (1); Natarajan, Sundararajan (2); Gravenkamp, Hauke (3)

1: University of Duisburg-Essen
2: Indian Institute of Technology Madras, India
3: International Centre for Numerical Methods in Engineering, Spain

08:30

Phase-field modeling of fracture proposed in [1] is a widely accepted approach in the community of fracture mechanics, as it intrinsically handles complex crack propagation, nucleation and branching phenomena. This diffusive fracture model leads to a non-convex optimization problem and demands a very fine mesh in the crack propagation region. In order to handle the former issue, staggered solution scheme has been extensively used in the literature, which results in convex elastic and phase-field sub-problems. On the other hand, the requirement of very fine mesh is handled either by initially pre-refining the mesh in the complete region of crack propagation or by using mesh adaptivity techniques.

In this regard, the scaled boundary finite element method (SBFEM) has proven to be a reliable technique for solving fracture problems on quadtree [2] and octree [3] meshes. Unlike in the standard finite element method, the elements with hanging nodes, arising in a quadtree or octree mesh, can be handled straightforwardly without any additional modification in SBFEM, thus leading to a more flexible adaptive solution technique. In the current work, a monolithic solution scheme for solving the coupled problem in the context of the SBFEM is proposed. This talk comprises a rigorous comparison of the accuracy and computational cost of both staggered and monolithic solution schemes.

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Acceleration of immersed computations of brittle phase-field fracture utilizing moment fitting schemes

Gorji, Mahan; Hosseini, Seyed Farhad; Sartorti, Roman; Radtke, Lars; Düster, Alexander 08:50
Hamburg University of Technology

Numerical simulations are very important in order to predict structural failure. Among various approaches, the phase-field modeling (PFM) seems to be very attractive. It is able to account for crack initiation, crack
propagation, dynamic crack branching, and more. It has been applied in different fields, e.g. brittle fracture, ductile fracture, mixed-mode fracture and dynamic fracture. The finite element method (FEM) is very popular for structural mechanical problems. It utilizes a boundary-conforming mesh to discretize the structure.
In recent years, immersed methods such as the finite cell method (FCM) have gained more attention in the scientific community. The FCM utilizes a Cartesian grid in order to discretize the structure, employing high-order hierarchical shape functions on each of the so-called ”finite cells”. Since the FCM mesh is no conforming to the geometry, the finite cells can be cut by the domain boundary, resulting in discontinuous integrands for the stiffness matrix and load vector. This issue is tackled by space-tree integration schemes, such as quadtrees (in 2D) and octrees (in 3D). Furthermore, the multi-level hp-method is applied to refine the FCM mesh towards the crack path.

The octree integration scheme is very robust and accurate. However, it leads a to huge amount of integration points and thus, is very expensive. On the other hand, moment fitting schemes are very promising, leading to a reduction of the integration effort. In particular, the non-negative moment fitting (NNMF) has been proven to be very efficient for nonlinear FCM computations. The idea is to derive an individual quadrature rule for each cut finite cell, where positivity of the weights is preserved. In this contribution, we employ the NNMF scheme in FCM simulations of brittle phase-field fracture with the aim of reducing the computational effort, while the accuracy is maintained. We study the proposed approach on numerical benchmarks first and finally apply it on brittle metal foams in order to predict strut failures.

Model-based analysis of surface roughness on fatigue processes

Yan, Sikang (1); Jawaid, Arsalan (1); Kerscher, Eberhard (1); Seewig, Jörg (1); Müller, Ralf (2) 09:10
1: RPTU Kaiserslautern-Landau
2: TU Darmstadt

In the last decade, the phase field method was developed to simulate fatigue fracture processes. The biggest advantage of phase field modeling is its unified framework, in which the entire fracture evolution from nucleation to propagation is covered. On the other hand, surface texture must be

considered in many areas of industry and research. In particular, surface roughness can fulfill complex functional requirements. For example, it is known that roughness has an essential impact on fatigue. In this work, we investigate how a phase field model for fatigue cracks can be used to incorporate roughness profiles. We also investigate the influences of different roughness profiles on fatigue processes with the help of the fatigue fracture phase field model. In all our studies, we leveraged roughness models.

Phase-field damage models for brutal crack growth: An adaptive time-discretization method

Rörentrop, Felix; Mosler, Jörn 09:30
TU Dortmund University

The modeling of brittle fracture has been an intensively researched topic for decades – both in the mechanical as well as in the mathematical community. In the past, the modeling of sharp cracks and the resulting free boundary problem posed significant numerical challenges. These difficulties have led to the rise of diffuse approximations in the sense of phase-field theories, which have become very popular, cf. [1].

Within this talk, the focus is on the numerical implementation of rate-independent phase-field damage models. This type of models is characterized by (incrementally defined) non-convex optimization problems. This non-convexity, in turn, leads to a discontinuous evolution of crack propagation in time. Different mathematical solution concepts have been proposed for such an evolution, cf. [2]. One mathematically sound concept is the adaptive time-discrete scheme proposed by Efendiev & Mielke, cf. [3]. Within this talk, an efficient and robust finite element implementation of framework [3] is outlined. A detailed analysis of the physics induced by the Efendiev & Mielke scheme is given.

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.
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[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, 2022

Efficient phase-field models for ductile fatigue fracture

Kalina, Martha; Kästner, Markus 09:50
TU Dresden

Phase-field modelling of fatigue fracture has been approached by many different models in recent years. Yet due to the high number of load cycles involved, computational time remains one of the main challenges, especially for fracture in ductile materials such as metals.

In this contribution, we revisit our efficient phase-field model for fatigue fracture [1] with a simplified consideration of cyclic plasticity. We combined the phase-field method for brittle fracture with the Local Strain Approach, a traditional fatigue concept from structural durability. It involves assumptions for the stress-strain behaviour including local plasticity and the damaging effect of load cycles, based on experimental material data.

Now, we improve the model by refining both the approximation of the stress-strain behaviour and the evaluation of the damaging effect of the load cycles with a new damage parameter. In a second step, we introduce a comprehensive phase-field model with elastic-plastic material law. This we use to evaluate the two efficient models with the simplified integration of plasticity. The range of application of the three models is discussed, compromising between accuracy and computational time.

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An eXtended Phase-Field Method for 2D Simulations of Fatigue Fracture Processes

Krüger, Christian; Curoșu, Verena; Loehnert, Stefan
TU Dresden

10:10

Due to its simplicity, the phase-field method is employed in many cases nowadays to solve fracture problems. It handles the phenomena of crack initiation, branching and merging implicitly without the necessity for further criteria or crack tracking algorithms. Applications to fatigue processes have shown that the method is able to reproduce fatigue characteristics like Wöhler-curves and the Paris-law. For this purpose, not only the stiffness of the material depending on the phase-field, but also the fracture toughness is degraded depending on the strain-history. However, besides these strengths, rather fine discretisations of the finite element mesh are necessary to represent the phase-field (particularly its high gradients) and the corresponding displacement jump adequately. Using classical Lagrange shape functions for the phase-field, the representation of the crack geometry becomes mesh dependent unless extremely fine meshes are employed.

To overcome these shortcomings, a combination of the phase-field method and the extended finite element method (XFEM) has been proposed. Within this extended phase-field method (XPFM) cracks can be represented with rather coarse meshes, independent of the element orientation. The major advantage of the novel method is that the number of unknowns can be reduced without any loss in accuracy, compared to the standard phase-field method. Especially with regard to fatigue simulations, the numerical effort decreases significantly. The basic idea of the XPFM is to use a transformed phase-field and an enriched displacement ansatz. The applied enrichment function directly depends on the transformed phase-field and allows for capturing the discontinuity of the displacement field across the crack represented only by the phase-field.

This contribution focuses on the treatment of fatigue fracture processes with the XPFM for the two-dimensional case. Special attention is drawn to some numerical issues, primarily to a non-standard, error-controlled quadrature scheme and to the control of convergence of the coupled staggered iteration and enrichment scheme update loop. Numerical examples of characteristic fatigue fracture problems are presented and compared to the solution within the standard phase-field approach.

S03.06: Damage and fracture mechanics 6

Date: March 21, 2024 14:00–16:00
Room: G22/013
Chair(s): Ricoeur, Andreas

Limitations of finite interface width in phase field simulations and solutions by the example of quasi-brittle damage evolution

Kurzeja, Patrick; Langenfeld, Kai; Mosler, Jörn
TU Dortmund University

14:00

Phase field descriptions for mechanical systems induce a finite, diffuse interface width that is often assumed or desired to be negligible [1,2,3]. On the one hand, the sharp-interface limit denotes the idealized reference for many applications, e.g., for crack propagation or phase transformations. On the other hand, however, the practical implementation yet requires to control a minimum width to be resolved by the numerical discretization. Properties such as Gamma convergence are hence often used as one test of suitable interfacial energies. Other properties such as derived stresses or final crack paths are often neglected, though, when checking for the convergence behavior of the phase field width - for instance, a possible interference between the interface width and the path of a freely evolving crack.

The present study examines the effect of the finite interface width on the physical behavior in the context of quasi-brittle damage evolution. It will be discussed by the examples of pre-damaged states as

well as freely evolving cracks. Particular attention is paid to the interaction of damage with geometric features. Limitations are identified in the form of interference with the physical response. While some studies employ the finite interface width of phase field descriptions solely for numerical regularization [1,3], others indicate finite interface widths to be a relevant origin for more complex physical behavior on smaller scales [4,5]. Variants of the phase field formulation are tested and discussed with respect to numerical practicability and their desired or undesired effects on the example simulations.

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On the influence of a nonlinear viscosity in a viscoelastic phase field model for fracture in ice

Sondershaus, Rabea (1); Humbert, Angelika (2,3); Müller, Ralf (1) 14:20

1: TU Darmstadt
2: Alfred Wegener Institute Bremerhaven
3: University of Bremen

Calving describes the break-off of icebergs from tidewater glaciers and ice shelves. It is a highly complex but poorly understood process in ice sheet dynamics and a physically based calving law has not yet been found. To obtain such a calving law the material behavior of polycrystalline ice needs to be considered as well as a fracture criterion.

Significant for glacier ice is its short-term elastic and long-term viscous behaviour, characterizing it as a viscoelastic material of Maxwell type. The viscous properties of ice can be described as a non-Newtonian fluid, known as Glen's flow law, leading to a stress-dependent viscosity. In addition, Glen's flow law also contains a rate factor that depends on the ice temperature, which can vary strongly over the ice thickness.

A well-established numerical approach to model fracture is the phase field method, which is based on a variational formulation of Griffith's theory. The state of the material, whether it is intact or broken, is represented using an additional continuous scalar field. This leads to a smeared-out crack representation but avoids the explicit modeling of crack faces and costly remeshing.

The phase field method for fracture is utilized in this contribution to simulate crack initiation and propagation in an ice shelf to study the effect of Glen's flow law on the fracture process. To describe the large deformations that occur due to the long-time viscous flow correctly, a nonlinear material description for viscoelasticity is used.

Simulations are conducted for a typically calving front geometry, where cracks are initiated by pinning points describing small areas where the normally floating ice shelf is grounded. We compare a finite viscoelastic Maxwell material with constant viscosity and a rate-dependent viscosity based on isothermal and parabolic temperature profiles to determine the impact of Glen's flow law.

An Enriched Phase-Field Approach to Fracture: Transformed Phase-Field Ansatz (Part 1)

Curoșu, Verena; Krüger, Christian; Löhnert, Stefan 14:40
TU Dresden

During the last years, the phase-field method for fracture has gained a lot of attention. It has become the most frequently used method for the simulation of quasi-static and dynamic fracture processes for brittle and ductile materials. Its biggest advantages are the simplicity of the implementation and the fact that it can capture crack propagation, branching, coalescence and initiation without the evaluation of additional criteria in a post-processing step. Another advantage compared to the very efficient XFEM/GFEM technique is that additional crack tracking algorithms and additional implicit or explicit representations of the crack geometry are not required. Despite its great success, the classical phase-field method has one severe disadvantage if standard Lagrange finite elements are employed. Due to the necessity of very fine meshes in the vicinity of an existing crack and its front, the computational effort is very high, which is amplified by the highly nonlinear behaviour even for the simulation of linear elastic fracture mechanics processes. For 3D simulations, in general high performance computing clusters are required. This makes the method rather unattractive for industrial applications.
Recently, an enriched/extended phase-field approach to fracture (XPFM) has been proposed [1], which combines the advantages of the XFEM/GFEM and those of the classical phase-field method and avoids this disadvantage. Within the XPFM, for the phase-field a transformed ansatz is used which resembles the analytical solution for a 1D phase-field problem. This transformed ansatz allows for significantly coarser meshes without increasing the number of degrees of freedom for each node. It is employed only in elements within which the phase-field exceeds a certain threshold. In all other elements a classical second order Lagrange ansatz function is employed. The transformed ansatz also allows for the reproduction of the crack within elements independent of the element orientation which is a prerequisite for the accurate representation of the crack also within a coarse mesh. In this presentation, the latest developments concerning the transformed phase-field ansatz are shown and properties are discussed. In the subsequent presentation (part 2) an improved variant of the displacement field enrichment is introduced and explained in detail.
[1] Loehnert, S.; Krüger, C.; Klempt, V.; Munk, L.: An enriched phase-field method for the efficient simulation of fracture processes. Computational Mechanics, vol. 71(5), pp. 1015-1039 (2023)

An Enriched Phase-Field Approach to Fracture: Enrichment of the Displacement Field (Part 2)

Curoșu, Verena; Krüger, Christian; Löhnert, Stefan 15:00
TU Dresden

The extended phase-field method (XPFM) combines the phase-field method for fracture with concepts from the extended/generalized finite element method. The concept aims to significantly reduce computational effort compared to the standard phase-field method. The advantages of not having to explicitly track the crack geometry and evaluate additional crack propagation criteria are retained.
In the preceding presentation (part 1), the transformed phase-field ansatz of the approach is discussed in detail. Beyond that, to be able to reproduce the high displacement gradients across the crack within the element, an enrichment of the displacement field is required. In the currently published methodology [1], to achieve this, the determination of a directional derivative perpendicular to the crack path was required. This direction was defined by the eigenvectors of the largest eigenvalues of a smooth projected strain field. Furthermore, to ensure C0-continuity across element edges within the enrichment function, the aforementioned derivative was smoothed out by employing a least-squares-fit. To prevent a relocation of the crack due to the projection procedure, the crack position was constrained at points, where the crack intersects the element edges.
Here, the approach is adjusted to avert the requirement for calculating these intersection points and the derivation direction. This enables more general applications and the extension to three dimensions. The main idea is to solve an inexpensive phase-field dependent Laplacian problem for each geometric direction on the domain of the reference element. The respective solution is a scalar field, which could be considered as modified, phase-field-dependent reference element coordinates which

are utilized in the enriched ansatz function for the displacement field. The advantage of a reference element-wise subproblem is that the mesh is identical for each element and the assembled global stiffness matrix and residual vector of each subproblem is known a priori. Additional effort solely lies in the correct inserting of phase-field values and the solving of the equation system for each enriched element.
In this presentation, the algorithmic procedure of the enrichment function calculation is shown and the enrichment and blending scheme is introduced. Furthermore, the application of the method to common academic examples for simulating fracture is shown.

[1] Loehnert, S.; Krüger, C.; Klempt, V.; Munk, L.: An enriched phase-field method for the efficient simulation of fracture processes. Computational Mechanics, vol. 71(5), pp. 1015-1039 (2023)

Prescribing traction-separation-laws to phase-field modelling of cohesive fracture

Lammen, Henning; Mosler, Jörn
TU Dortmund University

15:20

Cohesive zone models are capable to model a large spectrum of problems in non-linear fracture mechanics. They are characterized by an interface energy depending on the displacement jump, e.g., the opening of the interface. This results in tractions across the not fully opened interface, i.e., so-called traction-separation-law.

Several phase field approaches to cohesive fracture have been published over the last decade. The approach by Conti et al. [1] and Freddi and Iurlano [2] is characterized by a rigorous Γ-Convergence proof. The approach was recently enhanced by Lammen et al. [3]. Within the talk, the main enhancements of [3] are discussed including a finite strain setting, the properties of the cohesive energy as well as the Microcrack-Closure-Reopening-effect. The focus, however, is on the incorporation of certain shapes of the traction-separation-laws within this framework, e.g., linear or exponenential softening.

[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.

[3] H. Lammen, S. Conti, J. Mosler, A finite deformation phase field model suitable for cohesive fracture, Journal of the Mechanics and Physics of Solids 178 (2023) 105349.

S03.07: Damage and fracture mechanics 7

Date: March 22, 2024 08:30–10:30
Room: G22/013
Chair(s): Aldakheel, Fadi

Numerical investigations on three-dimensional metal cutting simulations within the Material Point Method employing the Johnson-Cook material law

Koßler, Marvin; Maassen, Sascha; Niekamp, Rainer; Schröder, Jörg
University of Duisburg-Essen

08:30

The Material Point Method (MPM) offers an alternative simulation approach, e.g., to the well-known Finite-Element-Method. Within this method, so-called material points are used to discretize the body while a compuational background grid is employed to solve the equations of interest, see [1]. The process of a MPM simulation within one time step can be divided into three steps, see also [2]. First, the quantities of the material points are mapped onto the grid nodes of the computational background grid, on which the degrees of freedom are then solved. With this in hand, the solution is mapped back to each material point individually. After each time step, the grid is reset as it does not carry any persistent information, enabling the material points to move independently of the background grid. As a result, mesh distortion in the context of huge deformations as in e.g. FEM simulations is completely avoided. This contribution presents simulations of metal cutting processes in both vertical and horizontal direction using three-dimensional models. The simulations incorporate the Johnson-Cook

material law, see [3], which accounts for plastic strain rates and the heat generated from plastic deformation during the cutting process. To achieve smoother solutions, the use of the grid-shift technique is suggested as introduced in [4].

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[1] D. Sulsky, Z. Chen, and H.L. Schreyer. A particle method for history-dependent materials. Computer Methods in Applied Mechanics and Engineering, 118(1-2):179–196, 1994.

[2] S.F. Maassen, R. Niekamp, J.A. Bergmann, F. Pöhl, J. Schröder, and P. Wiederkehr. Modeling of the Split-Hopkinson-Pressure-Bar experiment with the explicit material point method. Computational Particle Mechanics, 9:153-166, 2022.

[3] G.R. Johnson and W.H. Cook. A constitutive model and data for metals subjected to large strains, high strain rates and high temperatures. Proceedings of the 7th International Symposium on Ballistics, volume 21, pages 541–547, 1983.

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Simulation of coated particles breakage using Discrete Element and Bonded Particle Method

Safdar, Wasif; Heinrich, Stefan; Düster, Alexander 08:50
Hamburg University of Technology

Ship collisions remain a significant contributor to accidents, leading to severe environmental repercussions such as oil spills from tanker vessels. Enhancing the crashworthiness of ship structural design is crucial in mitigating these risks. One promising strategy involves incorporating granular material into the double hull structure, leveraging particle breakage to absorb kinetic energy and shift the load from the outer to the inner hull [1]. To optimize kinetic energy absorption and evaluate their effectiveness as crash absorbers, particles can be coated with environmentally friendly materials [2]. However, the mechanical behavior is contingent on the specific coating material, posing a challenge in establishing a numerical simulation model.
This study employs an open-source Discrete Element Method (DEM) code, MUSEN [3], to numerically model coated particles. This approach can be expanded using the Bonded Particle Method (BPM) to simulate particle breakage by solid bridges [4]. Given that the model involves both particles and bonds, the complexity of parameters increases, along with computational time. Consequently, a robust methodology is essential to characterize mechanical behavior irrespective of the coating material type, while also minimizing simulation time. An optimised DEM model is compared with experimental results from multi-particle compression tests to assess its capability in describing mechanical behavior at the multi-particle scale. Additionally, Finite Element Method (FEM) simulations are compared with DEM to delineate differences between the two approaches. The findings from these 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] 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.

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Brittle fracture investigation in a coupled peridynamic and classical elasticity model

Pernatii, Anna (1); Gabbert, Ulrich (1); Willberg, Christian (2); Hesse, Jan-Timo (2)
1: Otto von Guericke University Magdeburg
2: German Aerospace Center (DLR)

09:10

The simulation of crack patterns, crack velocities, and dissipated energies is a challenging task. Peridynamics has been proven to be a powerful tool addressing all these problems, including crack propagation, crack branching, its velocity and delamination, etc. It is a non-local theory where material points interact with points (called bonds) within a continuous neighborhood in a specific range, called horizon. Damages are considered in a constitutive model by allowing bonds to break when they are reach a predefined limit. Thus, Peridynamics is capable of accurate dynamic fracture analysis. The theory also allows the capture of damage on different scales, for instance, microbranching phenomena.

Typically, for complex problems Peridynamics is solved numerically. This numerical approximation is based on material point interactions. These implementations require a high spatial resolution for adequate representation of the damaged material behavior, which is related to the high computational costs. Additionally, because of the non-local nature of Peridynamics there are difficulties in applying the classical local initial and boundary conditions. This leads to the idea of coupling relatively expensive Peridynamics with a finite element method to reduce the computational efforts and also try to solve the boundary condition problem. If the whole domain can be divided into two subdomains, the area where the fracture is expected should be modeled with the Peridynamics and the rest – with finite elements. Because, of the high resolution needed to describe cracks, the problems occurring in the undamaged region won't matter.

Some coupled concepts were already investigated in previous works in a contest of damage-free dynamic problems with high-frequency excitement, and reflected waves were detected as a reason for the different wave dispersion parameters of both theories. The present work proposes an investigation of the influence of wave propagations on the fracture process, as well as on crack patterns and their velocities. The strategy is implemented in 2D, and the calibration of model parameters is also provided.

Peridynamic computations of wave propagation and dynamic fracture

Partmann, Kai; Weinberg, Kerstin
University of Siegen

09:30

Peridynamics describes the material in a nonlocal form and is well suited for dynamic fracture simulations. However, one significant effect regarding dynamic fracture is the correct handling of elastic deformation, like the pressure and tension waves inside a body, due to dynamic boundary conditions like an impact or impulse. Many peridynamic material formulations have been developed, and each has different advantages and challenges. The bond-based and continuum-kinematics-based formulations can handle wave propagation correctly but suffer from the surface effect. The non-ordinary state-based correspondence formulation does not suffer from the surface effect and models wave propagation with perfect accuracy. However, the correspondence models exhibit instabilities due to zero-energy modes and need stabilization, especially when dealing with cracks. The bond-associated non-ordinary state-based model emerges as a promising formulation that does not need stabilization. We demonstrate the differences between these formulations using wave propagation and dynamic fracture examples and compare various numerical results to analytical solutions.

Physics-based machine learning for computational fracture mechanics

Aldakheel, Fadi (1); Elsayed, Elsayed S. (1); Weeger, Oliver (2)
1: Leibniz University Hannover
2: TU Darmstadt

09:50

Physics-based machine learning leverages the strengths of both physics-based numerical simulation and data-driven approaches. By combining the flexibility and efficiency of state-of-the-art ML such

as deep learning with the rigor of classical continuum mechanical and thermodynamical models and numerical methods, accurate and fast predictions can be obtained in a reliable and robust manner. This hybrid approach opens up great potential for solving the current challenges in computational solid mechanics.

The current work introduces feedforward neural networks that enforce physics in a strong form to tackle computational fracture mechanics problems. Our proposed model undergoes training with various load sequences and is then evaluated for its capacity in both interpolation and extrapolation.

S04: Structural mechanics

Organizer(s): Klinkel, Sven *(RWTH Aachen Universtity)*
Freitag, Steffen *(Karlsruhe Institute of Technology)*

S04.01: Various topics in Structural mechanics

Date: March 19, 2024 08:30–10:30
Room: G26/H1
Chair(s): Klinkel, Sven

Remeshing in the Finite Cell Method for different types of geometry descriptions

Sartorti, Roman; Düster, Alexander 08:30
Hamburg University of Technology

The finite cell method (FCM) is one among different immersed domain methods. In contrast to standard Finite Element Methods the discretization does not need to conform to the boundary. Typically, a Cartesian mesh is generated and the domain boundaries are considered during the set up of the element/cell matrices. Therefore, the FCM is especially well suited for complex geometries such as, for example, foams where the geometry stems from CT-scans. Cells that are cut by the domain boundary are typically prone to large distortions and have negative impact on the condition of the global system matrix. This can be problematic, especially for finite strain analysis because the incremental/iterative solution procedure may not converge after a certain deformation state due to mesh distortions. To heal the largely distorted cells, in previous publications [1,2] remeshing has been applied.

To this end only triangulated surfaces were considered in the remeshing process so far. In the present study we examine the latest developments in the remeshing procedure to extend the applicability of other geometry descriptions, such as voxel models or level set functions.

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[2] Garhuom, W., Hubrich, S., Radtke, L., Düster, A.: A remeshing approach for the finite cell method applied to problems with large deformations. Proceedings in Applied Mathematics and Mechanics 21, 202100047 (2021) https://doi.org/10.1002/pamm.202100047

Immersed isogeometric analysis with boundary-conformal quadrature for large deformation problems

Elbadry, Yusuf T. (1); Antolin, Pablo (2); Weeger, Oliver (1) 08:50
1: TU Darmstadt
2: EPFL, Switzerland

Numerical simulation of complex geometries can be an expensive and time-consuming undertaking, in particular due to the lengthy preparation of geometry for meshing and the meshing process [1]. This problem becomes more apparent in cases of large deformation problems, where intermediate solution steps are necessary to achieve convergence. Various techniques were suggested to tackle this problem, including extended finite element, meshless, Fourier transform and immersed boundary methods. Immersed boundary methods [2] rely on embedding the physical domain into a Cartesian grid of finite elements and resolving the geometry only by adaptive numerical integration schemes. However, the accuracy, robustness, and efficiency of immersed or cut cell approaches depends crucially on the integration technique applied on cut cells.

In this work, we utilize an innovative algorithm for boundary-conformal quadrature that relies on a high-order reparameterization of trimmed elements [3] to address elasticity problems. We accomplish this using spline-based immersed isogeometric analysis, which eliminates the need for body conformal finite element mesh. The Gauss points on trimmed elements are obtained through a NURBS

reparameterization of the physical subdomains of the Cartesian grid to ensure precision integration with minimal quadrature points. This guarantees precise integration with minimal quadrature points. The 2D plate with hole problem serves as a benchmark problem for comparing the algorithm with conformal isogeometric analysis and the finite cell method. The results demonstrate that the adopted boundary conformal immersed Isogeometric analysis converges with optimal rates, thus demonstrating the efficiency and the precision of the method.

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On the importance of exact geometry representation for shell geometries with highly changing curvature

Dornisch, Wolfgang; Azizi, Nima 09:10
BTU Cottbus-Senftenberg

Since the early beginnings of isogeometric analysis in 2005, the exact representation of the geometry has been promoted as one of the main advantages. In more recent works, the high continuity enabled by spline basis functions is identified as main reason for the higher accuracy of IGA computations in comparison to standard finite element computations. In this contribution, we want to study the influence of the consideration of the exact geometry in detail for shell geometries with highly changing curvature. We compare a state-of-the-art isogeometric Reissner-Mindlin shell formulation to a high-order spectral finite shell element formulation. The geometry of the spectral shell elements is derived from the exact NURBS geometry by placing the nodes exactly on the physical domain and using the exact normal vectors at these nodes as nodal director vectors. Apart from this exact determination of nodal values, standard Lagrange basis functions are used to interpolate the geometry, the unknowns and the Jacobian. Since in spectral elements Gauss-Lobatto-Legendre quadrature is used, integration points and nodal points coincide. Thus, the physical coordinates are exact in all integration points, but all quantities based on derivatives of the shape functions, such as curvature and Jacobian, are approximations. As a third option a recently published intermediate option is studied. There the geometry including Jacobian is interpolated by the NURBS basis functions and thus exact, while the unknowns are interpolated by SEM basis functions. In the studied standard shell benchmark examples, the differences between all three considered formulations are very small. Here obviously, only the difference in the continuity between SEM and NURBS basis functions influences the obtained accuracy related to number of elements or degrees of freedom. The consideration of the NURBS geometry within the SEM elements slightly improves accuracy. However, if we study examples with arbitrarily changing curvature, a different picture is revealed. Surprisingly, for strongly changing curvature, the best results are obtained by the pure SEM formulation, which is not based on the exact geometry. The numerical results clearly show that even for highly changing curvature the exact representation of geometry is not important to obtain high precision results.

A scaled boundary shell formulation in isogeometric analysis for static and dynamic analysis

Reichle, Mathias; Hellers, Anna; Klinkel, Sven 09:30
RWTH Aachen University

In modern applications of computer-aided design (CAD) for the analysis of shell structures, isogeometric analysis is a powerful tool that integrates both design and analysis. An exact geometry description and a straightforward computation without loss of information are advantageous, especially for shell

structures such as roofs, satellite hulls, or car bodies. In addition, the scaled boundary method provides a scale separation with a semi-analytical solution procedure to consider a three-dimensional linear elastic constitutive law.

The presented approach deals with a scaled boundary solid shell formulation in the framework of isogeometric analysis. The formulation utilizes a normal scaling strategy which scales the shell along its normal vector at each point on the discretized bottom surface. This is fundamentally different from the well-known radial scaling strategy, where each point on the problem domain is obtained from a fixed scaling center. This results in a separation of the analysis into an in-plane direction and a scaling (normal) direction. By introducing the scaling, a scaled boundary differential equation is derived that is dependent on the scaling parameter only. Choosing a proper set of conditions, the differential equation can be solved by a Padé expansion. While the in-plane direction is solved in a weak sense, the thickness direction along the normal vector can be solved analytically resulting in a semi-analytical procedure. The isogeometric description of the CAD structure inherently yields the exact normal vector, its derivatives and a higher order continuity throughout the structure. Herein, the focus is on the solution technique in the thickness direction and the challenges are addressed. The power of the formulation is outlined in several numerical examples of static and dynamic analysis and a comparison to shell formulations in literature is provided.

The Mixed Displacement Method to Avoid Shear Locking in Problems in Elasticity

Vinod Kumar Mitruka, Tarun Kumar Mitruka; Bischoff, Manfred 09:50
University of Stuttgart

Over the last five to seven decades, in the context of the finite element method (FEM), geometric and material locking problems have been tackled by various methodologies. For instance, reduced integration, enhanced assumed strain method, assumed natural strain method, discrete strain gap method, B-bar method, and some other mixed methods have grown popular in this regard. Even though these methods work well to obtain locking-free finite elements, with growing diversification of discretization techniques, their extensions are rather not straightforward. In other words, the development of these unlocking methods has to be revisited while using, for example, isogeometric analysis (IGA), collocation methods, meshless methods, or the virtual element method. With the motivation of arriving at an unlocking scheme that works directly, independent of the element shape, polynomial order, and discretization scheme, Bieber et al. (2018) developed the *mixed displacement* (MD)*method,* which can be treated as an equivalent of the discrete strain gap method rewritten within a variational framework. In a sense, locking is avoided on a theoretical level before discretization. It includes adding extra degrees of freedom satisfying a chosen kinematic law incorporated in a mixed sense. Originally, the MD method was developed to address transverse shear locking in linear shear-deformable beams and plates and membrane locking in non-linear Kirchhoff-Love shell elements. Regardless of its straightforward implementation aspects, the MD method poses the challenge of handling certain constraints that are to be imposed on the additional degrees of freedom. Furthermore, the kinematic law chosen to handle membrane locking in Kirchhoff-Love shells, which could also be used for solid elements to manage in-plane shear locking, involves a second derivative, which supposedly increases the continuity requirement between the elements.

In this work, an overview of the above-mentioned MD method to mitigate the locking characteristics is provided. This is followed by a discussion of the extension of the MD method to geometrically linear and non-linear 2D and 3D solid elements. Moreover, recent investigations to lower the continuity requirement to the one needed by the primal formulation will be discussed. Afterwards, a methodology to treat the additional constraints is commented on. Numerical examples demonstrating the locking-free characteristics of the proposed methodology will be addressed as well. Here, the examples are examined in the context of FEM and IGA. The main focus will be on alleviating the shear locking phenomenon in solid elements with the MD method.

Simulation of Axisymmetric Problems Using the Petrov-Galerkin Finite Element Method

Zähringer, Felix; Betsch, Peter 10:10
Karlsruhe Institute of Technology

It is well known that in Finite Element (FE) simulations, the selected mesh has a strong influence on the quality of the results. Especially in the case of highly distorted meshes, large discrepancies between the numerical and the analytical solution can be observed. This effect is also evident when simulating axisymmetric problems, which is usually done using special FE formulations. 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 sensitive behavior.
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.
In several works (cf. [1], [2], [3]), Petrov-Galerkin FE formulations have been proposed for the simulation of linear elastic solids. Numerical investigations show that these elements have advantageous properties when simulations are performed with distorted meshes. In this contribution, it is analyzed to what extent the proposed concepts can be transferred to FE formulations for axisymmetric solids.

References

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[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: Various topics in Structural mechanics

Date: March 19, 2024 16:30–18:30
Room: G26/H1
Chair(s): Dornisch, Wolfgang

Analysis and Simulation of curved hoses under internal pressure - 3D continuum models

Hoesch, Quirin (1,2); Roller, Michael (1); Schneider-Jung, Fabio-Julian (1); Linn, Joachim (1); Müller, Ralf (2) 16:30
1: Fraunhofer ITWM
2: TU Darmstadt

A digital simulation tool, which is real-time capable and nevertheless physically correct, is required for the virtual safeguarding of vehicle cables, hoses or entire cable harnesses. For this purpose the structural-mechanical model and its mathematical formulation are crucial. It has been shown that geometrically exact rods are very suitable for such application cases. However, when the hoses are preformed and subjected to internal pressure, deformation behavior occurs that cannot be easily predicted using rod theory. Therefore, a finely resolved 3D continuum model is used to reproduce the real behavior of a curved hose under internal pressure as accurate as possible. With such a model all known effects like pressure dependent bending stiffness, radial expansion, axial shortening, cross-sectional deformation, as well as a curvature dependent force, also known as the Bourdon-Effect, could be simulated.

In this work, we focus on the Bourdon-Effect by simulating two simplified models. A full torus and a quarter torus. For an inflated full torus, the Bourdon-Effect can be observed by the fact that the radius of curvature increases in addition to the expansion of the cross-sectional radius. In the case of

a quarter torus, which is a simple example of a curved hose, the Bourdon-Effect can be observed by the tendency to straighten out under internal pressure. Furthermore it is detected for curved hoses, that the non-constant distribution of the poloidal (hoop) stress over the cross-section leads to an ovalisation behavior. In addition, the model of a quarter torus is extended to a more complex model with straight hose sections at both ends.

Finally we discuss how far this contribution is already able to identify the deformation behavior of preformed, pressurised hoses.

Influence of support conditions for violin plates in experimental modal analysis
Rauh, Benedikt; Akar, Özge; Willner, Kai
FAU Erlangen-Nürnberg
16:50

When it comes to studying the structural dynamic behavior, the violin proves to be a highly versatile subject as it encompasses various effects within a single structure. Exploring this musical instrument entails addressing uncertainties associated with natural materials, geometric nonlinearities, numerous interfaces, and the radiation of sound. However, two of the primary components of the violin, the top and the bottom plate, are delicate and lightweight structures that exhibit low frequency bending modes. Consequently, identifying modal parameters using experimental modal analysis proves to be quite difficult, particularly with regards to the support concepts employed, as they can significantly impact the modal behavior of the structures. To shed light on this matter, our research involves conducting experimental modal analyses on both the top and bottom plates. Various support structures, such as soft foams and elastic bands, are utilized during the experiments and the results are compared. The primary objective is to enhance our understanding of how different support conditions impact the measurement outcomes. This knowledge will enable us to make accurate statements regarding experimental modal analysis of violin structures, which in turn will aid future investigations aimed at optimizing the violin crafting process.

Approximate dual basis functions for mass lumping within explicit IGA simulations
Held, Susanne (1); Eisenträger, Sascha (2); Dornisch, Wolfgang (1)
1: BTU Cottbus-Senftenberg
2: Otto von Guericke University Magdeburg
17:10

Isogeometric analysis (IGA) utilizes shape functions that are directly derived from the CAD model. In contrast to the conventional Finite Element Method (FEM), which typically relies on Lagrange basis functions, IGA commonly employs Non-Uniform Rational B-Splines (NURBS) and other types of splines. For structures subjected to static or dynamic loads, IGA ensures highly accurate computations for a relatively low number of elements, as elevating the order of NURBS basis functions improves the convergence rate.

However, this precision comes at the cost of having mass matrices with large bandwidths, leading to an increased computational effort, especially in explicit dynamics, where a large number of time steps is usually required. To tackle this efficiency issue, mass lumping techniques are commonly employed to obtain diagonal mass matrices, simplifying the inversion process to a reciprocal operation. Although several lumping schemes have been derived in the literature, the row-sum technique is often favored. However, it has been primarily invented for standard FEM requirements. Unfortunately, when higher polynomial orders are in use, these simplistic approaches deteriorate the attainable convergence rates of IGA. Hence, developing a lumping scheme specifically tailored to higher order spline-based IGA formulations becomes imperative for efficient explicit dynamic computations.

This study proposes the usage of approximate dual test functions (AD) for B-Spline and NURBS-based IGA, while the shape functions remain unchanged. Implementing dual test functions, the Bubnov-Galerkin formulation is transformed into a Petrov-Galerkin formulation, resulting in a non-symmetric stiffness matrix and, as a consequence of duality, consistent diagonal mass matrix. The AD approach approximates this behavior and leads to banded, but diagonally dominant mass matrices. Hence,

additional row-sum lumping is applied to obtain diagonal mass matrices. The induced error is significantly smaller compared to the accuracy loss experienced when applying mass lumping within a conventional IGA formulation.

Implementing this approach into existing IGA codes is a seamless process, facilitated by the use of a transformation operator. This operator serves as the link between the shape functions and their respective dual functions, enabling the straightforward generation of dual matrices. Numerical examples demonstrate that the lumped AD scheme enables nearly equivalent efficiency to conventional lumping techniques while simultaneously achieving an accuracy level that is similar to a consistent IGA formulation.

On the potential of approximate dual basis functions towards efficient mixed plate formulations in isogeometric analysis

Stammen, Lisa; Dornisch, Wolfgang
BTU Cottbus-Senftenberg

17:30

Within isogeometric analysis, non-uniform rational B-splines (NURBS) are used as shape functions and trial functions, in order to obtain highly accurate results, as these functions offer high inter-element continuity and the ability to represent the geometry exactly during the analysis procedure.

Mixed formulations are employed in order to alleviate locking effects that occur both in standard finite element methods and within isogeometric analysis. Therefore, different fields of unknowns are approximated independently. This also allows to adapt the interpolation orders separately, which counteracts locking effects that are introduced due to non-matching interpolation orders in the shear strain equation. As the higher number of parameters increases the computational effort, static condensation of the additionally introduced variables is desirable. Depending on the structure of the system matrix, this can be computationally expensive. In NURBS-based isogeometric analysis, this has to be performed on patch level, if the continuity of the relevant basis functions is higher than C^0. In order to decrease the costs for the inversion of the relevant submatrix to a minimum, lumping it into a diagonal matrix could be considered. To reduce the error introduced thereby, approximate dual basis functions can be selected for the test functions corresponding to these parameters. This approach can be especially efficient in the scope of nonlinear analysis, where iterative solution methods such as the Newton-Raphson procedure require an inversion of the system matrix in every step.

In this contribution, the potential of approximate dual basis functions towards efficient mixed plate formulations is studied within an isogeometric framework. Therefore, a mixed plate formulation with deformations and shear forces as independent fields is derived and the interpolation orders are adapted accordingly, in order to alleviate occurring locking effects. Using approximate dual basis functions for the interpolation of the shear parameters enables an efficient static condensation of these parameters. The benefits of this proposed procedure are studied for a benchmark problem by comparing the accuracy of results and the computational effort to those of a standard isogeometric plate formulation.

A closed-form approach on mode III loading of thin layers

Rheinschmidt, Florian (1); Adam, Valentin (1); Weißgraeber, Philipp (2); Rosendahl, Philipp L. (1)
1: TU Darmstadt
2: University of Rostock

17:50

Weak interface models are a potent tool to capture both deformations and stresses and energy release rates for adhesives or other weak layers between stiffer joints. While the energy release rate for both mode I and II is rendered well, a fast and efficient model, capturing mode III loading of the weak layer is lacking. The present study addresses this research gap by bringing forward a closed form analytical model for out-of-plane bended weak interface specimen.

The classical approach of weak interface models as outline by Volkersen [1] and Goland and Reissner [2] is not applicable in case of loading the specimen with out-of-plane bending. Tackling these difficulties, the present approach uses the principle of minimum potential energy in combination with the calculus of variations to derive the governing equations for an arbitrarily loaded weak interface

specimen. This model renders stresses and displacements in a very good agreement with numerical reference solutions and is highly efficient and reduces the numerical costs for parameter studies and the evaluation of experiments. This enables one, to measure the mode III energy release rate from a J-integral based evaluation of this physical quantity. Thus, this model allows a fast determination of the mode III fracture toughness from out-of-plane loaded double cantilever beam tests for adhesives or from rotated propagation saw tests for faceted and porous weak layers in stratified snowpacks.

[1] Volkersen, O. Die Nietkraftverteilung in Zugbeanspruchten Nietverbindungen mit konstanten Laschenquerschnitten, *Luftfahrtforschung*, 15:41-47, 1938

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S04.03: Various topics in Structural mechanics

Date: March 20, 2024 08:30–09:30
Room: G26/H1
Chair(s): Weeger, Oliver
Klinkel, Sven

Kinematic Hardening and Size Effects in Elastoplastic Nonlinear Timoshenko Beams

Gärtner, Til (1,2); van den Boom, S.J. (2); Weerheijm, J. (1); Sluys, L.J. (1) 08:30
1: TU Delft
2: Netherlands Institute for Applied Scientific Research (TNO)

Architected materials, like lattice structures composed of beams, have attracted increasing interest due to their unique properties. For instance, auxetic materials, which exhibit a negative Poisson's ratio, offer potential advantages for impact protection, including increased indentation resistance, fracture toughness, and energy adsorption. These properties appear promising in the search for lighter materials for impact protection. In literature, numerous architectures have been proposed to achieve auxetic properties, however with limited insight into nonlinear effects. Efficient numerical models are required to capture geometric and material nonlinearities and to explore the behavior of different architectures.

Nonlinear Timoshenko beams can be used to model lattice materials. These beams commonly account only for linear material behavior. Recently Herrnböck et al. [1,2] have developed a framework to determine the yield surface and hardening tensor in the full six-dimensional cross-sectional force and moment space. This extension to include plasticity in the modelling of beams allows the efficient simulation of elastoplastic lattice structures under large deformation in impact scenarios. In their framework, they describe the scaling of the yield surface in relation to the macroscopic geometric size and the scaling of the hardening tensor in relation to the microscopic hardening properties. For the study of different lattice architectures under finite deformation, the scaling of the hardening tensor with respect to the macroscopic geometric size is of further interest and has not been discussed so far.

The objective of this research is to examine macroscopic geometrical scaling effects of the hardening tensor in the full six-dimensional cross-sectional force and moment space. A numerical framework is established for conducting elastic analysis of single non-linear Timoshenko beams and multi-beam structures. The framework is then extended to include the yield surface of Herrnböck et al. [1] for ideal plasticity. Careful consideration is given to meshing of the beams and to load-stepping in relation to the explicit return mapping scheme. Kinematic hardening, as described by Herrnböck et al. [2], is subsequently added to the analyses. The effects of geometric scale on the hardening tensor are explained and a method to adapt the hardening tensor in order to account for scale effects is presented. The investigations are conducted on both single cantilever beams and lattice architectures for auxetic metamaterials.

[1] Herrnböck et al., Comput Mech. 67 (2021), pp. 723–742.

[2] Herrnböck et al., Comput Mech. 71 (2022), pp. 1–24.

Isotropic growth model for generalised scaled boundary isogeometric analysis on slender structures

Spahn, Florian; Kolisch, Florian; Praster, Maximilian; Rosado Balmayor, Elizabeth; Klinkel, Sven 08:50
RWTH Aachen University

The contribution is concerned with a numerical method to model growth for naturally grown structures like plants or trees. In the last decade, building botany has evolved as a new discipline of living construction design in modern architecture [1]. Therefore, trees are lead in the right shape to join as a load-bearing structure. The structural system consists of curved, slender, and naturally grown geometries interconnecting with conventional structural parts. The individual structural elements consist of thin, curved branches. For structural analysis, geometric features such as curvature or bifurcations exhibit unique static capabilities. It is crucial to transfer these geometries into the calculation model accurately. The structure can be accurately depicted through three-dimensional scanning techniques, such as 3D laser scanning. A fundamental model as a point cloud via surface data acquisition is created in this process. From the point cloud data, a NURBS model can be extracted. The model exists as a 2D surface within a 3D space. Using scaled boundary isogeometric analysis (SBIGA) [2,3] approaches, surface NURBS models can be directly applied for structural analysis. When conventional SBIGA is used for slender structures, obtuse-angled polyhedral patches can occur, leading to numerical condition problems. Therefore, a novel generalised scaled boundary isogeometric analysis (GSBIGA) approach is introduced. This new method employs a scaling centre line instead of a scaling centre point. For a description of the leading process, a growth simulation is done.

The present approach is based on [4] and applied to wooden growth. The deformation gradient is split multiplicatively into an elastic and a growth part. Therefore, an elastic deformation-free intermediate configuration is considered. The formulation for modelling volumetric growth is located on the kinematic level. Specific basic growth mechanisms apply to tissues and wood, such as shape adaption and remodelling. Therefore, a formulation for modelling volumetric growth is combined with the novel GSBIGA approach. This allows the modelling of the growth of slender geometries, such as living structures or tissues, using image-based data.

[1] F. Ludwig et al. Living systems: Designing growth in baubotanik. *Architectural Design*, 2012.

[2] M. Chasapi et al. Isogeometric analysis of 3D solids in boundary representation for problems in nonlinear solid mechanics and structural dynamics. *IJNME*, 2021.

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Physics-enhanced neural networks for material modeling in beam theory

Schommartz, Jasper Ole; Alzate Cobo, Juan Camilo; Klein, Dominik; Weeger, Oliver 09:10
TU Darmstadt

A machine learning based methodology for modeling and calibration of hyperelastic beams subjected to large strains and large deformation is presented. The approach exploits the high-dimensional interpolation capabilities of neural networks and captures the nonlinear material response directly through strain and stress measures making numerical integration over the cross-section obsolete. Building on prior physical knowledge, the model is enhanced with thermodynamic consistency, stress and energy normalization, as well as symmetry for beams where the material distribution in the cross-section is point symmetric to the center of mass. An extension is presented, which enables parameterization with the radius of the cross-section. Calibration and testing data was generated with an implementation of the geometrically exact beam model and by solving the cross-sectional warping problem with the finite element method. Strain measures were sampled using a concentric sampling strategy, which ensures physical admissibility and sensibility of every data point. The physics-enhanced model achieves excellent accuracy on univariate and mixed load paths with strain

amplitudes smaller 0.5 and good accuracy for even larger strains. The radius-parameterized model enables good approximations for circular beams with radius to length ratios greater 0.04.

S04.04: Various topics in Structural mechanics

Date: March 20, 2024 14:00–16:00
Room: G26/H1
Chair(s): Fries, Thomas-Peter

Inverse Problem for Parameterizing Nonlinear Elastic Bending Behavior for Cable Simulation

Zhao, Tian (1,2); Schneider-Jung, Fabio (1); Linn, Joachim (1); Müller, Ralf (2) 14:00
1: Fraunhofer ITWM
2: TU Darmstadt

For slender structures such as cables and hoses, the theory of geometrically exact Cosserat rods provides a suitable framework for an efficient modelling and simulation [1]. Often, their bending behavior is characterized by a linear elastic constitutive law. This is sufficient for many cases with simple cable structures, however, for more complex cables e.g. a high-voltage cable, a linear elastic model for bending deformations might not cover the real behavior. In general, nonlinear as well as inelastic effects occur. Here, we only consider nonlinear elastic bending behavior, incorporating inelastic deformations by considering pre-curvature.

In our recent work [2], we propose an iterative method for the forward simulation of nonlinear elastic behavior. In each iteration, the algorithmic bending stiffness constants are updated according to a given bending stiffness characteristic, and the static equilibrium is calculated by energy minimization. The iteration is repeated until the convergence of the cable state is achieved. To identify the bending stiffness characteristic from measured values of real cables, we formulate the corresponding inverse problem.

Recently, we enhanced the inverse problem such that not only the bending stiffness characteristic is determined but also the specimen's pre-curvature, which might vary along the rod. We validate this approach with numeric examples and apply it to experimental data.

[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.

Test Rig for Validating the Integrated Motion Measurement of Flexible Beams

Kohl, Michael; Györfi, Benedikt; Wagner, Jörg Friedrich 14:40
University of Stuttgart

The root of integrated motion measurement (IMM) is integrated navigation with inertial sensors combined with, e.g., a satellite navigation receiver. Accordingly, IMM makes also use of the specific advantages of complementary sensors and blends them in a filter algorithm. To meet requirements in advanced motion measurements for structural health monitoring or for structural control purposes, the approach of a single rigid body like in classical navigation no longer holds for IMM. As a solution, additional degrees of freedom (DOFs) are introduced for the moving structure which represent deformations and allow the navigated body to be treated as a flexible structure.

To cover a variety of flexible deformation shapes, a sufficient number of distributed inertial sensors is required. To restrict accumulating errors of these sensors, an aiding by additional structural measurements is necessary. The signals of the inertial sensors and the aiding measurements are fused by an extended Kalman filter (EKF) to obtain an optimal estimation of the usual navigation states, extended by the deformation variables.

This contribution presents the preparation of the experimental validation of an IMM system for a flexible structure, which represents an idealization of a wing or rotor blade by a movable beam. For that, the mechanical and electrical setup of a test rig is described. Furthermore, the simulation of the test configuration is discussed, i.e. the model of a test beam with a variety of distributed sensors for generating artificial measurements as test reference. Finally, for an optimal sensor placement, the two methods of effective independence and maximization of modal energy are compared for different amounts of additional flexible DOFs.

Simultaneous solution of implicitly defined curved, linear Timoshenko beams in two-dimensional bulk domains

Kaiser, Michael Wolfgang; Fries, Thomas-Peter
Graz University of Technology

15:00

A mechanical model and a corresponding finite element method (FEM) for the *simultaneous* solution of *infinitely many* curved, linear Timoshenko beams which are embedded in a two-dimensional background domain are presented. Classically, *one* geometry is defined explicitly by curvilinear coordinates. In the proposed model, however, the beam's centre axes are implied by *all* level sets of a scalar function in a bulk domain, thus the geometry description is implicit. The coordinate-free formulation of the governing equations is achieved using the Tangential Differential Calculus and is, therefore, independent of curvilinear coordinates. Similar models for*one single* structure are formulated for curved beams in three-dimensions in [1], for Reissner-Mindlin shells in [2], and for non-linear ropes and membranes in [3]. For the numerical analysis, the two-dimensional bulk domain is discretized by higher-order elements for the simultaneous solution of *all* beams in the bulk domain. The endpoints of the beams coincide with the boundary of the bulk domain, hence, no cut elements occur and (essential) boundary conditions can be enforced strongly. This approach is a significant extension of the method for ropes and membranes proposed by the authors in [4] to structures with bending actions, i.e., the curved Timoshenko beams. Higher-order convergence studies of numerical examples, based on the residual errors in the force and moment equilibrium, ensure the validity of this method and confirm optimal convergence rates. To further verify the proposed method, the stored elastic energy integrated over all beams is compared to results obtained by the classical FEM in successive simulations for individual level sets.

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[2] D. Schöllhammer and T.P. Fries, Reissner-Mindlin shell theory based on tangential differential calculus, Comp. Methods Appl. Mech. Engrg., 2019
[3] T.P. Fries and D. Schöllhammer, A unified finite strain theory for membranes and ropes. Comput. Methods Appl. Mech. Engrg., 2020.
[4] T.P. Fries and M.W. Kaiser, On the simultaneous solution of structural membranes on all level sets within a bulk domain, Comp. Methods Appl. Mech. Engrg., 2023.

A direct peridynamic-type beam theory

Naumenko, Konstantin; Yang, Zhenghao
Otto von Guericke University Magdeburg

15:20

In the past decade non-local structural mechanics theories, e.g. theories of beams, have become increasingly important due to applications in micro- and nanometer scale components, composites with high contrast in properties and laminates with extremely thin layers. A class of weakly nonlocal beam theories is developed in the literature by including higher order deformation gradients as arguments of the strain energy density. The aim of this presentation is to discuss a family of beam theories by introducing long-range force and moment interactions as well as conjugate deformation measures. Starting from the classical concept of the deformable line balance equations for the linear and the angular momentum are formulated. The cross sections of the deformable line are assumed to behave like rigid bodies, i.e. translations and rotations degrees of freedom are considered. Applying the principle of virtual work, as well as concepts of absorbed and supplied work, integral deformation

measures, constitutive equations and boundary conditions are introduced. With special constitutive assumptions for the force and moment vectors a peridynamic theory for elastic beams is developed. For several boundary conditions closed form analytical solutions to peridynamic equations of motion are derived providing the deflection as well as internal force and moment densities as functions of the beam coordinate and time. As the peridynamic horizon size approaches zero the results converge to those of the classical first order shear deformation beam theory.

A variational approach to inelastic Cosserat rods in the plane 15:40

Schneider-Jung, Fabio (1); Manfredo, Davide (1); Dörlich, Vanessa (1); Arnold, Martin (2); Linn, Joachim (1)
1: Fraunhofer ITWM
2: Martin Luther University Halle-Wittenberg

Stable equilibrium configurations of elastic Cosserat rods can be computed by minimizing their elastic energy. In our contribution, we outline a variational procedure that provides stable solutions of quasistatic sequential plane deformations of Cosserat rods possessing inelastic constitutive properties in an analogous manner.
As a concrete example, we demonstrate our approach with a Cosserat rod model, where the constitutive law yields the bending moment as a rate independent functional of the current bending curvature and its history in terms of a Prandtl-Ishlinskii (PI) hysteresis operator. Besides outlining the theoretical approach for both the continuum and the discrete rod model, we show some illustrative numerical examples of plane bending with the resulting hysteretic effects.
We also indicate how the model ingredients of the PI hysteresis operator can be identified from results of cyclic plane bending experiments, with composite cables as a concrete application example.

S04.05: Various topics in Structural mechanics

Date: March 20, 2024 16:30–18:30
Room: G26/H1
Chair(s): Weinberg, Kerstin
Ricken, Tim

Lattice structures as an energy-absorbing component for impact loads 16:30

Bieler, Sören; Weinberg, Kerstin
University of Siegen

Lattice microstructures can be produced quickly using additive manufacturing because the fast advancement of 3D printing technology and the associated high print resolutions make it possible to produce structures of any scale. For example, these structures are attractive in many areas to save weight due to their excellent stiffness-to-weight ratio. Due to the elastic and plastic deformation of the lattices under load, lattice structures also have excellent energy absorption properties. The energy-absorbing properties of the structure depend on various factors such as the choice of material, printing process, and layout. The absorption properties of such structures are of particular interest, especially in the case of impact loads.

In this contribution, we present an experimental investigation of energy-damping lattices, especially the octet structure. The test specimens are created using a 3D printer that works according to the stereolithography process with up to 35 µm resolutions. Different volume fractions of the structure are examined for their energy-absorbing properties. To this end, the specimens are examined using the split Hopkinson pressure bar test to apply an impact load. Conclusions can be derived about the energy absorption of the specimen from the strain pulses measured in the system.

Investigating Auxetic Elements to Enhance Energy Absorption in Flexible Structures: An Integrated Experimental and Numerical Approach

Pi Savall, Berta; Seyedpour, Seyed Morteza; Ricken, Tim 16:50
University of Stuttgart

In the search for innovative solutions for lightweight materials with high absorption capacity, this research specifically investigates the hyperelastic behaviour of auxetic flexible structures. Auxetic structures, which are characterised by a negative Poisson's ratio, offer high energy absorption and low weight, making them particularly suitable for lightweight applications such as aerospace. This study, which combines experimental and numerical approaches, provides insights into the mechanical behaviour of flexible, additively manufactured auxetic structures to improve energy absorption.

In the experimental phase, the strains and their derivatives in flexible, planar structures are accurately measured using a digital image correlation (DIC) system during tensile tests. The analysis focuses on how the dynamic Poisson's ratio is affected during the test. The numerical aspect uses a finite element simulation with the hyperelastic Mooney-Rivlin material model to characterise these structures at the macro level. The comparison between experimental and simulation results shows a coherent correlation, which proves their reliability. Based on this simulation, the strains are compared with the experimental results for validation and the stresses and absorbed energy are calculated.

Based on this, 3D structures are analysed. In an experimental study, flexible 3D-printed samples of thin-walled tubes surrounded by an auxetic shell are used for compression tests. The results show that the inclusion of auxetic structures leads to higher energy absorption compared to cylindrical walls of the same mass.

Numerical and Experimental Modeling of the Mechanical Behavior of Syntactic Foam (lightweight aggregates - Aluminum 2024)

Sadeghpourhaji, Reza; Mohammadkhah, Melika; Klinge, Sandra 17:10
TU Berlin

Metal matrix composite foams (MMSF) are versatile lightweight materials with exceptional properties that offer a promising solution for addressing climate change, particularly in reducing carbon emissions in transportation, and find relevance in various industries due to their remarkable energy absorption capabilities. However, the relatively high cost associated with MMSF fabrication methods and additive particles presents a significant challenge, limiting their widespread development and application.

This contribution addresses this challenge by proposing the use of cost-effective porous particles, such as perlite, Lightweight Expanded Clay Aggregate (LECA), and pumice, with properties resembling hollow shells. Despite their abundant availability, there is a surprising lack of research on these affordable and lightweight particles. To bridge this gap, the current work focuses on fabricating lightweight syntactic foam structures using the vacuum casting method and conducting both numerical and experimental analyses of their mechanical properties. Finite Element Method (FEM) is used for micromechanical analysis to comprehensively evaluate their mechanical properties. The computational model results are compared with experimental data, obtained through precision manufacturing of MMSF samples via a vacuum casting process, followed by quasi-static pressure tests.

In the study, lightweight aggregates (expanded perlite, LECA, and pumice) are investigated as fillers to produce metal matrix syntactic foams with low density (1.09-2.05 g/cm^3) through the vacuum casting method. These commercial materials with porous structures are available at low cost. No unwanted penetration or chemical reactions between the aggregate particles and the aluminum 2024 matrix are observed. The resulting syntactic foam samples exhibit an overall porosity of 62.52%, surpassing previous syntactic foams. Uniaxial compressive tests under quasi-static conditions revealed promising mechanical properties for Perlite/Al2024, LECA/Al2024, and Pumice/Al2024 combined foams. The average plateau stress is 18.36, 25.10, and 40.43 MPa, respectively, with corresponding densification strains of 65%, 69%, and 60%. These structures proved to be excellent energy absorbers, demonstrating high energy absorption efficiency with averages of 66%, 70.50%, and 79%.

The comprehensive investigation of MMSFs presented in this study contributes to the evolution of sustainable and high-performance materials, paving the way for enhanced efficiency, safety, and environmental responsibility in various industries.

Simulations of superelastic lattice materials manufactured by additive manufacturing using a hypoelastic material model

Schasching, Marius M. (1); Červinek, Ondřej (2); Munhowen, Tim (1); Koutný, Daniel (2); Pettermann, Heinz E. (1); Todt, Melanie (1)
1: TU Wien
2: Brno University of Technology, Czech Republic

17:30

Lattice materials offer great potentials in engineering applications as their internal architecture significantly influences their effective mechanical response. With progressing additive manufacturing techniques, lattice materials with man-tailored mechanical properties are easily manufactured. In combination with superelastic parent materials, such as NiTi alloys, lattice materials allow for large deformation states without reaching the yield limit of the parent material. The reversibility of the deformations due to the phase-transformation of the parent material is of interest in any application relying on re-usability or where the initial state must be restored.

An adequate prediction of the mechanical response of lattice materials requires models to properly capture both the deformation mechanisms of the internal architecture and the material response of the parent material. The available material models often represent an idealized form of superelastic material behavior, from which the experimentally measured response of real materials often deviate. The modeling of lattice materials by means of the Finite Element Method is often more efficient when beam elements are used instead of continuum elements. For beam elements, uniaxial constitutive material models are sufficient.

To give adequate predictions using beam-based models, a user defined material model is implemented to account for the superelastic constitutive behavior of an additive manufactured material. The uniaxial material model is based on a hypoelastic constitutive law using the UHYPEL user subroutine of ABAQUS 2023/Standard (*Dassault Systèmes Simulia Corp., Providence, RI, USA*). To facilitate correct predictions of unloading/reloading loops at intermediate (transformation) strains, case distinction is utilized. A least squares fit is used to obtain a smooth function for representing the mechanical response of the parent material obtained by experimental tests. Additionally, a piecewise linear function is fitted by hand. The intersection points of the piecewise linear functions are further used as input for the standard superelastic model readily available only for continuum elements in ABAQUS. To study the capabilities of the beam-based models, a comparison is made for various lattices using the hypoelastic models developed for beam elements and the standard superelastic model for continuum elements.

The results show that the beam-based models in combination with the hypoelastic material models are suitable for describing the effective mechanical response of the additive manufactured lattice materials. The numerical efficiency allows for the employment of the developments in a wide variety of applications, including large scale lattice materials.

Acknowledgement
The project has been funded by European Union Program Horizon Europe under grant agreement no. 101079091.

Tuning the buckling behaviour of slender, material extrusion manufactured collinear stayed polymer lattices

Ou, Yating; Köllner, Anton; Völlmecke, Christina
TU Berlin

17:50

Lattice structures are widely used nowadays because of their high strength-to-weight ratio. However, they are particularly sensitive to elastic buckling failure at low relative densities. A novel type of lightweight and high-performance, collinear polymer lattice with the concept of stayed slender

columns will be presented, which is fabricated using extrusion–based additive manufacturing technology [1]. The buckling and post-buckling behaviour of the stayed unit cells (UCs) and two-dimensional lattices is investigated analytically and experimentally

The analytical study is performed reminiscent of [2] with a three degree of freedom system based on the general theory of elastic stability [3]. The total potential energy is expressed by the strain energy and the work done by load. The strain energy of the structures is described using the Rayleigh-Ritz method, where the displacements are approximated by three generalised coordinates. Equilibrium states are determined through solving a set of nonlinear algebraic equations within a Python-based module 'pyfurc' in which the stability of equilibrium is also evaluated [4]. Parametric studies of perfect and imperfect systems are performed, including geometric parameters and material characteristics.

Compression tests are conducted, where the UCs and lattices are loaded under applied end-shortening with a simple support to observe the buckling behaviour. The experimental results indicate that the ultimate load of the UCs and lattices with stays increases significantly compared to those without stays, which is achieved by adding minor weight.

The concept of stayed columns significantly improves the compressive strength and buckling behaviour of stayed lattices compared with conventional lattices. The combination of experiments and simulations opens the door to optimizing design parameters in the future, promising more efficient and functional lattice structures.

[1] Ou, Y., Köllner, A., Dönitz, A., & Richter, T. E. (2023). Material extrusion additive manufacturing of novel lightweight collinear stayed polymer lattices [Unpublished manuscript].

[2] Zschernack, C., Wadee, M. A., & Völlmecke, C. (2016). Nonlinear buckling of fibre-reinforced unit cells of lattice materials. *Composite Structures*, *136*, 217-228.

[3] Thompson JMT, Hunt GW. A general theory of elastic stability. London: Wiley; 1973.

[4] Klunkean/pyfurc: Auto-07P made accessible through python. https://github.com/klunkean/pyfurc

A robust finite strain isogeometric solid-beam element towards simulations of microlattice structured Li-ion battery electrodes

Shafqat, Abdullah; Weeger, Oliver; Xu, Bai-Xiang 18:10
TU Darmstadt

In this work, an efficient and robust isogeometric three-dimensional solid-beam finite element is developed for large deformations and finite rotations with merely displacements as degrees of freedom. The finite strain theory and hyperelastic constitutive models are considered and B-Spline and NURBS are employed for the finite element discretization. Similar to finite elements based on Lagrange polynomials, also NURBS-based formulations are affected by the non-physical phenomena of locking, which constrains the field variables and negatively impacts the solution accuracy, and deteriorates convergence behavior. To avoid this problem within the context of a Solid-Beam formulation, the Assumed Natural Strain (ANS) method is applied to alleviate membrane and transversal shear locking and the Enhanced Assumed Strain (EAS) method against Poisson thickness locking. Furthermore, the Mixed Integration Point (MIP) method is employed to make the formulation more efficient and robust. The proposed novel isogeometric solid-beam element is tested on several single-patch and multi-patch benchmark problems, and it is validated against classical continuum finite elements and isoparametric solid-beam elements. The results show that the proposed formulation can alleviate the locking effects and significantly improve the performance of the isogeometric solid-beam element.

The developed isogeometric solid-beam finite element [1] would be then coupled with Fick's second law of diffusion to develop the isogeometric chemo-mechanics solid-beam element with concentration as additional degrees of freedom. Variation of Gibbs (chemical) and elastic free energy functions would help to derive the chemical potential and the hyperelastic constitutive models which are induced by the two-way coupling. With the developed element, efficient and accurate prediction of lattice-based Li-ion battery electrodes can be achieved. The proposed solid-beam element inherits both the merits of solid elements e.g., flexible boundary conditions and of the beam elements i.e., higher computational efficiency.

[1] A.Shafqat, O.Weeger, B.Xu, A robust finite strain isogeometric solid-beam element (submitted)

S04.06: Various topics in Structural mechanics

Date: March 21, 2024 08:30–10:30
Room: G26/H1
Chair(s): Freitag, Steffen
Altay, Okyay

Physics-based machine learning model for the manufacturing of thermoplastic composites

Hürkamp, André 08:30
TU Braunschweig

The process combination of thermoforming thermoplastic fibre-reinforced sheets and injection moulding of thermoplastic polymers enables the production of thermoplastic composites with proper mechanical properties and geometrical complexity. However, the resulting mechanical properties of the composite structure such as fibre orientation and strength depend largely on the local conditions during the manufacturing process. In particular, the draping of the sheet and the temperature during manufacturing have a significant influence. Furthermore, shrinkage and temperature-induced deformations cause a deflection of the produced part. To compensate this deflection, process parameters need to be optimized as well as the mould geometry needs to be adapted. Available numerical tools are able to simulate the injection moulding process as well as the resulting deflection. However, the desired optimisation task requires many queries and hence many evaluations of the numerical simulation, which is computationally expensive. In order to reduce the computational effort, a physics-based surrogate model is presented that combines Proper Orthogonal Decomposition (POD) and Machine Learning. Based on a snapshot approach the most significant POD modes are extracted. In this case, a decomposition of spatial and process-dependent functions can be obtained. By doing so, the predicted result can be written as a series expansion. In order to capture a wide range of parameter combinations, the corresponding POD coefficients need to be computed for arbitrary parameter inputs. Machine Learning, i.e. artificial neural networks, is well suited to act as a nonlinear function between input and desired output (deflection).

In this work, a network architecture for the estimation of the deflection of thermoplastic composites is presented, where the series expansion is used as an additional constraint in the objective function. In this way, it is possible to compute physical reliable deflections for a multi-dimensional parameter input within seconds or even shorter. Such a model can further serve as additional assistance during operation when it is connected directly to the process parameters of the production system.

Artificial neural networks for structural damage detection and localization

Freitag, Steffen; Volovikova, Anastasiia 08:50
Karlsruhe Institute of Technology

Structural health monitoring (SHM) can help to assess the state and the reliability during the life-time of a structure. In SHM, measured signals of the structure are compared with the corresponding reference signals obtained from the pristine state and adequate damage indicators are defined, e.g. based on displacements, eigenfrequencies or guided waves. The damage indicators can be utilized for damage detection, damage localization and damage size prediction. In this presentation, an artificial neural network (ANN) concept is introduced, where the damage indicators are used as input of feedforward networks. A first classifier ANN is trained to decide if the structure is damaged or not. In a second step, the damage position is localized by a regression ANN. The concept is tested using the Open Guided Wave dataset, where a carbon-fiber composite plate stiffened by an omega stringer is investigated. The classifier ANN is set up by a weighting of the training error with respect to the damage size to achieve an acceptable false alarm rate (ca. 0.1) and an increasing probability of detection with increasing damage size. By a statistical evaluation of the classifier ANN predictions, the minimal detectable damage size for a given probability (e.g. 0.9) is obtained. For the damage localization, the regression ANN prediction (position of the damage) of different sender receiver signal path

is combined and a probabilistic filter is applied to focus on the damage positions with the highest concentrations. These results are finally used to compute the probability of correct localization for a defined precision range.

Advanced discretization techniques for hyperelastic physics-augmented neural networks

Franke, Marlon (1); Klein, Dominik K. (2); Weeger, Oliver (2); Betsch, Peter (1) 09:10

1: Karlsruhe Institute of Technology
2: TU Darmstadt

In the present work, advanced discretization techniques are tailored to hyperelastic physics-augmented neural networks. In particular neural network based constitutive models are designed which fulfill all relevant mechanical conditions of hyperelasticity by construction. The computation of derivatives for these neural network based constitutive models parallels that of analytical models; however, the complexity of these computations is heightened. This motivates to tailor advanced discretization methods for neural network based constitutive models, to arrive at compact mathematical formulations and convenient implementations with superior stability and robustness in static and dynamic analysis. In particular, the proposed neural network based framework allows for convenient mixed Hu-Washizu like finite element formulations applicable to nearly incompressible material behavior. A key feature of this work is a tailored energy-momentum scheme for time discretization, which allows for energy and momentum preserving dynamical simulations. Both, the mixed formulation and the energy-momentum discretization are applied in finite element analysis. For this, a hyperelastic physics-augmented neural network model is calibrated to data generated by an analytical potential. The proposed discretization techniques are examined for their stability and robustness properties in representative finite element simulations. All of these observations illustrate that, from a formal perspective, neural networks fundamentally operate as mathematical functions. As such, they can be applied in numerical methods as straightforwardly as analytical constitutive models. Nevertheless, their special structure suggests to tailor advanced discretization methods, to arrive at compact mathematical formulations and convenient implementations.

Physics-Informed Neural Networks for Material Model Calibration

Anton, David (1); Wessels, Henning (1); Henkes, Alexander (2); Römer, Ulrich (1) 09:30

1: TU Braunschweig
2: ETH Zurich

The identification of material parameters occurring in material models is essential for structural health monitoring. 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. Knowing the current condition of the building structures can help prevent disasters and extend service life.

We developed a parametric physics-informed neural network (PINN) for the calibration of material models from full-field displacement data measured by digital image correlation. In an offline-phase, the PINN is trained to learn a parameterized solution of the underlying parametric partial differential equation without the need for training data. We demonstrate the ability of the parametric PINN to act as a surrogate in a least-squares based material model calibration. In order to quantify the uncertainty, we further use the parametric PINN with Markov-Chain-Monte-Carlo based Bayesian inference. Even with artificially noise data, the calibration produces good results for reasonable material parameter ranges. Especially in iterative and sampling based methods, parametric PINN have the advantage that model evaluation is very cheap compared to, e.g., the Finite Element Method. Thus, information on the material condition can be provided in near real-time in the online-phase. Moreover, PINN use a continuous ansatz and thereby avoid the need to interpolate between sensor and simulation domain and vice versa.

Advanced Parameter Identification for Structural Steel Modeling: Integrating Multiple Load Protocols with Convolutional Neural Networks

Altay, Okyay (1); Lignos, Dimitrios (2)
1: RWTH Aachen University
2: EPFL, Switzerland

09:50

Robust prediction of material responses in constitutive models relies on their input parameters. Young's modulus and other parameters, reflecting physical characteristics, are typically obtained directly through physical experiments. However, these models also depend on parameters essential for internal computations, where their correlation with measured responses is often complex and not easily interpreted.

Our study addresses this challenge by introducing a data-driven approach using convolutional neural networks (CNNs) to identify and calibrate parameters for structural steel. Unlike existing solutions that use feedforward neural networks, CNNs allow for the processing and interpretation of multiple strain-based uniaxial protocols simultaneously, revealing the underlying material behavior. We enhance the process by coupling two networks, thereby simplifying training, and increasing accuracy in parameter identification. The primary network maps stress data to parameters, a traditionally complex task. The secondary network, a surrogate of the constitutive model, maps in tandem these parameters back to stress responses. This dual-network approach establishes an efficient and well-posed training environment.

To validate our method, we apply it to the Updated Voce-Chaboche (UVC) model, which requires precise calibration for simulating the inelastic behavior of metals. We generate training data by simulating steel material responses with parameters obtained by Latin hypercube sampling. Ten different uniaxial strain-based protocols are utilized that feature monotonic, cyclic, and incrementally increasing amplitudes. Once the surrogate model is trained to map the stress responses from the parameters, the training of the primary CNN is efficiently conducted with the same data. After training, the elastic modulus and yield stress are identified from measured stress responses with eight additional parameters crucial for modeling of isotropic and kinematic hardening effects. A comparison with the experimental results assumes the effectiveness of the proposed approach, as the UVC model accurately replicates the experimental responses with the identified parameters. The results suggest that, within the sampled parameter space, without retraining, the method is applicable to various structural steels, regardless of their composition and form.

In conclusion, our method seamlessly integrates multiple load protocols, demonstrating well-posed and versatile applicability. This approach holds significant promise for the advancement of structural steel modeling, which could influence future research and practical applications.

Physics informed neural networks in structural dynamics

Polydoras, Vasileios; Tandale, Saurabh Balkrishna; Stoffel, Marcus
RWTH Aachen University

10:10

The aim of this study is to enhance the computational efficiency and convergence characteristics of Finite Element Method (FEM) simulations through the integration of Artificial Neural Networks (ANNs) in dynamically loaded structures, where the influence of inertia effects is considered.

Machine learning has emerged as a helpful tool in accelerating the computation time of structural mechanics simulations. Artificial Neural Networks (ANNs) have been incorporated into Finite Element Method (FEM) simulations, through material law replacement to speed up the simulation time, leading to the so-called intelligent elements [1]. Physics Informed Neural Networks (PINNS) have also found application in structural mechanics, exhibiting the objective of learning the underlying physics [2].

With the present study, we introduce an ANN-based method to approximate the non-linear material behavior. This computation is essential for the computation of the internal forces within each element in 1D and 2D dynamic FEM simulation. The learning algorithm employed in this study is also trying to learn the underlying physics by including physical constraints of the corresponding material law in the loss function.

Therefore, the objective of this study is to introduce enhanced beam and plate elements by replacing physical non-linearities with ANN based method. Following this intention, it is investigated how the neural network enhanced approach can accelerate the simulation speed of the overall domain and improve the convergence of the Boundary Value Problem with physical non-linearities.

1. Stoffel M., Bamer F., Markert B., Artificial neural networks and intelligent finite elements in non-linear structural mechanics, Thin-Walled Structures, 131, 102-106, 2018.

2. Ehsan Haghighat, Maziar Raissi, Adrian Moure, Hector Gomez, Ruben Juanes, A physics-informed deep learning framework for inversion and surrogate modeling in solid mechanics, Computer Methods in Applied Mechanics and Engineering, Volume 379, 2021, 113741, ISSN 0045-7825.

S04.07: Various topics in Structural mechanics

Date: March 21, 2024 14:00–16:00
Room: G26/H1
Chair(s): Zilian, Andreas
Wulfinghoff, Stephan

Simulation of viscoplastic structures under material uncertainties using time-separated stochastic mechanics

Geisler, Hendrik (1,2); Junker, Philipp (1,2) 14:00
1: Leibniz University Hannover
2: IRTG 2657: Computational Mechanics Techniques in High Dimensions

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 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 the application of the time-separated stochastic mechanics to the simulation of viscoplastic structures under material uncertainties. Comparisons to the Monte-Carlo method showcase its exceptional accuracy at a fraction of the computational cost.

Numerical analysis of the stress-based formulation of linear elasticity

Sky, Adam; Zilian, Andreas 14:20
University of Luxembourg

The Beltrami-Michell equations of linear elasticity differ from the Navier-Cauchy equations, in that the primary field in former equations is the stress tensor rather than the displacement vector. Consequently, the equations can be used for circumstances where the displacement field is not of interest, for example in design, or when increased smoothness of the solution of the stress tensor is desired. In this work we explore the stress-based Beltrami-Michell equations for linear isotropic materials. We introduce the equations in modern tensor notation and investigate their limitations. Further, we demonstrate how to symmetrise and stabilise their weak formulation, complemented by existence and uniqueness proofs. With latter at hand, we construct a conforming finite element discretisation of the equations, avoiding the need for intermediate stress functions. Finally, we present some numerical examples.

Variational three-field reduced order modeling for nearly incompressible materials

Shamim, Muhammad Babar; Wulfinghoff, Stephan 14:40
Kiel University

This research introduces an innovative strategy for developing a reduced-order model (ROM) designed specifically for nearly incompressible materials experiencing large deformations. The methodology adopts a three field variational approach to effectively capture the intricate behavior of such materials. In constructing the ROM, the initial step involves solving the full-scale model using the finite element method (FEM), wherein snapshots of the displacement field are recorded and organized into a snapshot matrix. Subsequently, the Proper Orthogonal Decomposition (POD) technique is applied to extract dominant modes, forming a condensed basis for the ROM.

Additionally, we address the pressure and volumetric deformation fields adeptly by incorporating the k-means algorithm for clustering. Leveraging a well-established three-field variational principle allows the seamless integration of clustered field variables into the ROM. To evaluate the efficiency of our proposed ROM, we conduct a comprehensive comparison between the ROM with and without clustering against the FEM solution. Our findings underscore the superior performance of the ROM with pressure clustering, especially when considering a restricted number of modes, typically fewer than 10 displacement modes. The validity of our results is confirmed through two standard examples: one involving a compressed block and another featuring Cook's membrane. In both scenarios, significant enhancements are achieved through the three-field mixed approach. These compelling outcomes emphasize the effectiveness of our ROM approach in accurately capturing nearly incompressible material behavior while reducing computational expenses.

Mitigation Techniques for Volumetric Locking in the Implicit Material Point Method (MPM)

Meyer, Julian; Kaliske, Michael 15:00
TU Dresden

The material point method (MPM) aims to avoid mesh distortion problems occurring in the commonly used Finite Element Method (FEM). To achieve this, the continuum is discretized as a set of material points, while the solution of the weak form of the underlying partial differential equations is conducted on an Eulerian background mesh. As this process works similar to FEM, the MPM also displays volumetric locking for near-incompressible materials. However, this also means that mitigation techniques developed for FEM can be adapted to the MPM. The main difficulty for this process lies in the higher-continuity basis functions, which are required in MPM to achieve reasonable results. This study first reviews the applicability of different locking techniques in MPM. Then, a framework for a locking-free implicit MPM is presented and validated using common tests investigating the locking behavior and stress oscillations. Finally, the presented methods are applied to a viscoelastic material model representing unvulcanized rubber to show the potential of MPM for tire molding simulations.

Stabilization-free Virtual Element Method for 3D Hyperelastic Applications

Xu, Bing-Bing; Wriggers, Peter 15:20
Leibniz University Hannover

The Virtual Element Method (VEM) can be regarded as a generalization of the classical finite element method (FEM) to general polygonal meshes. In the prior studies of the VEM, a stabilization term is required in order to ensure that the global stiffness matrix has the correct rank. In this work, we present a stabilization-free Virtual Element Method for hyperelastic materials in 3D. The main idea of the stabilization-free approach is to use an enhanced approximation space to compute a higher-order polynomial projection of the gradient. In this work, the formulation of the stabilization-free VEM for 3D hyper-elastic materials is given. Some numerical examples are given to compare the accuracy of the stabilization-free VEM with the conventional VEM.

Mathematical Foundation of the Master-Slave Elimination for Arbitrary Nonlinear Multi-Point Constraints

Boungard, Jonas (1); Wackerfuß, Jens (1); Ortleb, Sigrun (2) 15:40
1: Institute of Structural Analysis, University of Kassel
2: Department of Mathematics, University of Kassel

Nonlinear multi-point constraints are essential in modeling various engineering problems, for example in the context of joints undergoing large rotations or coupling of different element types in finite element analysis. Constraints can be handled by Lagrange multipliers, the penalty method and the master-slave elimination. The master-slave elimination satisfies the constraints exactly and reduces the dimension of the resulting system of equations which is particularly advantageous when a large number of constraints have to be considered. However, the existing schemes in literature are limited to linear constraints. Therefore, the authors introduced an extension of the method to arbitrary nonlinear constraints [1]. In contrast, Lagrange multipliers satisfy the constraints exactly but introduce additional unknowns and lead to a saddle point structure of the resulting system of equations. The penalty method does not alter the underlying structure of the resulting system of equations. However, small penalty factors lead to a violation of the constraints and large penalty factors, while approximately satisfying the constraints, worsen the condition number of the resulting matrix.

A mathematically rigorous derivation of the new master-slave elimination scheme for arbitrary nonlinear multi-point constraints is presented. Starting point is the *optimization problem with constraints*. It is transformed into a *modified optimization problem without constraints* using the *implicit function theorem*. In order to perform this transformation, an appropriate set of slave degrees of freedom (dofs) has to be chosen in such a way that the Jacobian of the constraints satisfies several conditions.

This has several implications on the implementation into a finite element code as well as the application of constraints in specific problems. The following challenges are addressed: The automatic selection of slave dofs (instead of a manual, error-prone selection by the user), the change of the slave dofs necessary in the context of large deformation scenarios and the handling of redundant and contradictory constraints. An algorithm for the selection of slave dofs in this context was developed in [2]. We illustrate the implications of the mathematical foundation on these problems with several numerical examples.

[1] Boungard, J. and Wackerfuß, J.: Master-slave elimination scheme for arbitrary nonlinear multi-point constraints. In: *Computational Mechanics* (under review)

[2] Boungard, J. and Wackerfuß, J.: *Identification, elimination and handling of redundant nonlinear multi-point constraints*. In preparation.

S04.08: Various topics in Structural mechanics

Date: March 21, 2024 17:40–18:40
Room: G26/H1
Chair(s): Hürkamp, André
Freitag, Steffen

Accelerating the design of the effective surface of pressing tools with probabilistic inverse modelling approaches

Hupfeld, Henning Karsten (1); Teshima, Yuta (2); Ali, Syed Sarim (1); Juraschek, Max (1); Dröder, Klaus (1); Herrmann, Christoph (1); Hürkamp, André (1) 17:40
1: TU Braunschweig
2: The University of Tokyo

In the design and production of press parts, the tool development process is an essential step. However, this is also a complex process. The accuracy requirements are high and it takes a lot of experience to accurately design the effective surface with respect to the multitude of physical, procedural and human influences. Thus, several iterations in the tool development process are usually required,

which is costly and can make the process a bottleneck in the product design cycles [1]. To accelerate this, we propose a diffusion model architecture [2] to inversely design the necessary effective tool surface given a desired geometry of the press part. This diffusion model is able to reduce the generalization issues of classical machine learning approaches by leveraging the attention mechanism both in the spatial and temporal dimension of the underlying forming process. The applicability of a similar diffusion model could already be shown for the inverse-design of metamaterials [3] and this publication further demonstrates that diffusion models can be a suitable model candidate for the inverse-design of 3D-geometries. For model training, Finite Element simulations that contain the time series of deformation states during the forming process were used. Furthermore, different geometry variations of part and tool as well as relevant press process parameters were used in the training. The results will be validated against simulation results computed by the commercial forming simulation software Autoform.

[1] Birkert, A.; Haage, S.; Straub, M. (2013). Umformtechnische Herstellung komplexer Karosserieteile. https://doi.org/10.1007/978-3-642-34670-5.
[2] Ho, J.; Chan, W.; Saharia, C.; Whang, J.; Gao, R.; Gritsenko, A.; Kingma, DP.; Poole, B.; Norouzi, M.; Fleet, DJ.; Salimans, T. (2022). Imagen Video: High Definition Video Generation with Diffusion Models. https://doi.org/10.48550/arXiv.2210.02303.
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Structural dynamics of a Scaled Trailer Model: Investigation of the Influence of Different Loading Variants

Volltrauer, Jan Markus (1); Buck, Fabian (1); Hetzler, Hartmut (2)
1: Daimler Truck AG, NVH Entire Vehicle
2: University of Kassel

18:00

Simulations play a pivotal role in streamlining the product development process, aiming to minimize the overall development time. A crucial prerequisite for effective simulations is the utilization of models that represent real-world dynamics. This study employs experimental modal analysis techniques to examine the structural dynamics of a scaled trailer model, focusing on its response under diverse loading configurations. The goal is to extrapolate these findings to real-life scenarios and develop a mechanical equivalent model capable of replicating the structural dynamics of the trailer under various loading conditions with a high degree of accuracy.

The scaled trailer model is designed to exhibit dynamic equivalence to a reduced-size trailer at a scale of 1:8. Consequently, the model's natural frequencies are eightfold higher than those of the full-sized counterpart. The accompanying test bench facilitates realistic excitation of the trailer at both the kingpin and axle. Given that the investigation focuses on examining the standalone trailer (without a tractor unit), a suspension featuring four springs has been developed, also serving the purpose of static load equalization.

The research systematically introduces alterations to the scaled model, encompassing diverse load variants, changes in load distribution, weight adjustments, and overall configuration modifications. This approach enables a thorough analysis of the individual and collective effects of these alterations on the structural behaviour of the trailer. Extracting key parameters such as natural frequencies, mode shapes, and damping ratios from experimentally determined frequency responses form the basis for in-depth analysis.

The investigation reveals that variations in loading conditions induce observable changes in the structural response of the trailer. Initial results emphasise the major effects of the coupling of load and centre of gravity position. The local stiffening resulting from the coupling of the load to the trailer structure illustrates how specific load configurations can lead to localized structural modifications. Additionally, the position of the centre of gravity emerges as a pivotal parameter influencing the overall dynamics of the trailer.

Future research will expand investigations by exploring an extensive range of loading conditions, encompassing variations in payload types, road courses, diverse excitation forces, and various load coupling methods. By implementing the relevant dynamic effects of the trailer loading into simulation models, this research is intended to make a scientific and practical contribution to the development and optimisation of semi-trailers and tractor units in the evolving transport landscape.

S04.09: Various topics in Structural mechanics

Date: March 22, 2024 08:30–10:30
Room: G26/H1
Chair(s): Völlmecke, Christina

Analytical considerations of the load-deflection behavior in fibers during a filament winding process

Steinweller, Christina; Hartmann, Stefan 08:30
Clausthal University of Technology

Filament winding is a process used to manufacture fiber composite structures, where a bundle of fibers is drawn through a thermoset resin-hardener bath and wound onto a mandrel. It is applied in the production of rotationally and non-rotationally symmetrical hollow vessels, for instance in the fabrication of pipes, tanks or pressure vessels, but also in prototype construction in the aerospace industry.
Of particular interest is the arising stress and strain state during the production process, which is significantly driven by the pre-stressed fiber tension. Therefore, analytical considerations of a wound cylinder are taken to estimate the stresses in fiber direction and the accompanying stresses in the radial direction (pressure on the mandrel).
Due to the cylindrical shape of the component, it is advisable to describe the occurring deformations and the equilibrium conditions in curvilinear coordinates. In a first approach, the material behavior of the glass-fibers is assumed to be of compressible Neo-Hookean type.
The equilibrium conditions formulate a boundary-value problem, which can numerically be solved under different boundary conditions. In addition, production-related influences such as the loss of frictional force due to the friction between the cylinder and the fiber (or between fibers with itself), and the winding angle are varied in order to analyze their influence on the stress state.

Computational Modeling of Concrete Composites with Short Shape Memory Alloys Fibers

Tabrizikahou, Alireza; Kuczma, Mieczysław 08:50
Poznan University of Technology, Poland

The application of fiber-reinforced concrete (FRC) in the construction sector is a developing area of study and application. Shape memory alloy (SMA) is one promising material for use as fibers in FRC due to its ability to revert to its original shape after deformation, a phenomenon known as the shape memory effect (SME). FRC may be pre-stressed and self-repaired by combining SMA with the SME characteristic. Nevertheless, modeling SMA-FRC using conventional finite element methods (FEM) is demanding. This paper presents an innovative technique for modeling SMA-FRC utilizing multiscale modeling. The article describes the methods for generating micromechanics, homogenization, boundary conditions, and coupling micro- and macro-models. The results demonstrate that employing multiscale modeling may significantly lower computing costs while presenting extra insights about the SMA-behavior FRCs on the microscale. The results also suggest that employing SMA fibers can generate sufficient pre-stressing forces in the concrete, improving the stiffness and durability of the concrete. Nevertheless, several parameters like fiber geometry, pull-out strength, SMA phase transformations, and crack progression are simplified in the article. The authors intend to resolve these limitations in further research and compare the findings to experimental data. The usage of SMA-FRC has significant potential for enhancing the durability and strength of concrete buildings, and the unique multiscale modeling technique given in this study can assist in the advancement of research in this sector.

Torwards a holistic simulation framework for the response of a multilayered pavement structure subjected to realistic tire loading

May, Marcel; Anantheswar, Atul; Wollny, Ines; Kaliske, Michael 09:10
TU Dresden

The current study introduces a framework for the realistic and computationally efficient modeling of layered, temperature-dependent, and inelastic pavements. The constitutive relationships of the several layers in the road superstructure account for large deformations resulting from tire rolling. The tire-pavement interaction is validated by tests conducted on real tires. The material formulations are embedded in a novel dynamic Arbitrary Lagrangian Eulerian (ALE) formulation, which significantly increased the speed and efficiency of the simulation compared to a traditional Lagrangian approach. This improvement stems from the need to discretize and simulate only the relevant mesh portion around the applied load. Notably, this eliminates the necessity for a cumbersome moving load formulation. The obtained results exhibit satisfactory agreement when compared to a conventional Lagrangian simulation incorporating a moving load [1].

REFERENCES

[1] Anantheswar, A.; Wollny, I. and Kaliske, M.: A dynamic ALE formulation for structures under moving loads. Computational Mechanics, 2023.

Additive Manufacturing in Structural Mechanics: Tackling Sustainable Development Goals through Cooperative Labwork

Völlmecke, Christina; Dönitz, Antonia; Panjalipoursangari, Narges; Ou, Yating 09:30
TU Berlin

Additive Manufacturing (AM) stands as a catalyst for fostering interdisciplinary cooperation in both research and teaching within the realm of structural mechanics. Our multidisciplinary team champions research-based teaching, emphasizing cooperative labwork and the integration of Sustainable Development Goals (SDGs), focusing on sustainable materials, gender and diversity. By bridging theoretical concepts with practical applications through AM, our approach contributes to transforming the educational and scientific landscape.

Engineering students frequently overlook the inherent interdisciplinarity embedded in structural mechanics projects due to the traditional isolation of modules in standard engineering curricula. This fragmentation impedes students' understanding of cross-disciplinary connections, as exemplified by the disparate focus of mechanics and experimental modules. To address this, our hands-on, teamwork approach actively engages students in tackling interdisciplinary applied mechanics challenges using additive manufacturing, experimental testing and open source simulation.

Our initiative extends beyond the confines of traditional engineering boundaries, fostering interdisciplinary research that encompasses cooperation with e.g. fungal based biotechnology or textile design. Examples will be presented. Embracing a multidisciplinary team, our approach empowers engineering students and early stage researchers to become adept problem solvers with a steadfast commitment to sustainability, gender and diversity and a comprehensive understanding of structural mechanics. This holistic and inclusive methodology promotes collaboration and cultivates a multifaceted approach to solving complex challenges of today's world.

Numerical Validation of an Innovative 3D Calculation Method of High-Rise Buildings under Consideration of Component and Soil Stiffness

Badr, Michael (1); Müllner, Herbert W. (2) 09:50
1: TU Wien
2: PORR Bau GmbH, Austria

The static design of skyscrapers is mostly based on finite element calculations of the supporting structure whereas 3d calculations are required to consider the influence of horizontal forces such as wind

loads and earthquake, respectively. In addition 2d calculations are performed to determine unfavorable internal force variables of carrying elements such as columns and walls, respectively. Nevertheless the comparison of these calculations of the same building shows differences up to 100 percent depending on the height of the building.

To investigate the column loads a research project in cooperation between Vienna University of Technology and PORR Bau GmbH has been performed. As a result an innovative calculation method for three-dimensional building models has finally been developed which is based on a stiffness combination vector that can be used independently of the program and free of the modeling quality of the responsible structural engineer. Furthermore, the bedding modulus for base slabs is varied within the limits specified by the soil survey by dividing the base slab into quadrants.

In this contribution a numerical validation of the innovative calculation method is carried out by means of approximately 200 simulations for two major projects in Vienna [1]. By comparison with the real building forces, which are based on measured in-situ strains [2], a clear identification of the stiffness combination vector for the load-bearing components is possible.

The calculation results obtained in this way for vertical, load-bearing concrete elements, such as columns and walls, show the smallest differences with the measurement results of the various buildings.

By applying the present stiffness combination vector to any building structure, it is thus possible to cover the nonlinear concrete properties (shrinkage, creep, concrete maturity) and the time-dependent effects (construction phases) with the help of a finite element model. By applying the innovative process to future construction projects, the probability of over- or under-sizing of supporting structures will be reduced.

[1] M. Badr: Numerical Validation of an Innovative 3D Calculation Method of High-Rise Buildings under Consideration of Component and Soil Stiffness, Master Thesis, Vienna University of Technology, 2023, in German.

[2] H.W. Müllner, W. Wallisch, P. Kremnitzer: Back Calculation of Internal Forces of Concrete Skyscrapers by means of In Situ Monitoring", PAMM – Proceedings in Applied Mathematics and Mechanics, 21 (2021), 1, https://doi.org/10.1002/pamm.202100045

Experimental Validation of an Innovative Method for Minimization of Deformation Tolerances of Reinforced Concrete Ceilings

Müllner, Herbert W. (1); Akyol, Sarah (1); Hofer, Peter (2) 10:10

1: PORR Bau GmbH, Austria
2: pde Integrale Planung GmbH, Austria

The static design of reinforced concrete ceilings is mostly based on finite element calculations. If the calculated deformation is too big, a superelevation is carried out in order to optimize the thickness of the ceiling. The superelevation is achieved by setting parts of the formwork a fixed amount higher than the edge areas of the ceilings before concreting.

In most cases, the superelevation is determined by the structural engineer as a part of the expected total deformation under consideration of a safety surcharge. However, because areas with less stress sink less strongly, this approach means that the superelevations are not dismantled there and the ceiling remains in an elevated position. In addition, climatic conditions and the construction phases are not taken into account in the calculations. This leads to problems in the subsequent finishing trades, for example the facade assembly or the installation of the floor pavement.

To investigate real ceiling deformations a research project in cooperation with the University of Applied Sciences in Vienna has been performed [1]. The goal was to determine the deformations of ceilings under consideration of formwork and ceiling support. Therefore, deformation measurements of twenty ceilings of a 88 m high office complex in Vienna has been performed between the day of production of the ceiling until six months afterwards in order to validate methods of the state of the art as well as to develop new methods for minimization of deformation tolerances of reinforced concrete slabs.

In this contribution a validation of various numerical methods such as [2] for the deformation of concrete slabs by means of measurement results is shown whereas the focus is on the multi-story support of ceilings which have not arrived the full Young's modulus.

The research project shall help to avoid damages and minimize the time effort of the subsequent finishing trades which still occur in current building projects.

[1] P. Hofer: Analysis of ceiling deformation in dependence on temperature, material development, stripping dates and the static system, Master Thesis, University of Applied Sciences, 2018, in German.

[2] T. M. Laggner, D. Schlicke, N. V. Tue, W.-D. Denk: Statische Analyse mit linear elastischen 3D-Gebäudemodellen, Beton- und Stahlbetonbau, 116 (2021), 360–369, in German.

S05: Oscillations

Organizer(s): Stender, Merten *(TU Berlin)*

S05.01: Oscillations (1)

Date: March 19, 2024 08:30–10:30
Room: G22/217
Chair(s): Stender, Merten

Experimental nonlinear modal analysis: its potential and recent advancements

Scheel, Maren 08:30
University of Stuttgart

Due to the demand for higher efficiency and light-weight design, nonlinear vibration phenomena occur in, for example, slender or jointed structures. To ensure safe operation, these nonlinearities must be considered when predicting vibrations. Besides powerful numerical tools, measurements are indispensable to verify these predictions and identify parameters of nonlinear models. However, the large variety of nonlinearities calls for nonlinear system identification methods that do not assume any a-priori functional form of the nonlinearity. One approach is to employ the concept of nonlinear vibration modes and to determine natural frequencies, damping ratios and modal deflection shapes as function of the vibration level. Hence, the widespread experimental modal analysis was recently extended to nonlinear systems. Being an experimental realization of the extended periodic motion concept, this method is suited for both stiffness and damping nonlinearities. The experimentally identified single nonlinear mode accurately describes forced responses around a well-separated resonance, i.e. is meaningful in the absence of strong modal interactions.

In the simplest realization, a single-point, single-frequency force is applied to the system to drive it to phase resonance and to track the system's backbone curve. The phase lag between force and response is controlled using a phase-locked loop controller. Once the controller is locked, the system vibrates in a steady state. Finally, amplitude-dependent modal properties are extracted from the steady-state measurement data. In the method's latest implementation, an adaptive filter is used to estimate the phase lag. In combination with a systematic tuning procedure of the control parameters, the measurement duration is substantially reduced compared to previous implementations. This tremendously reduces the experimental effort and minimizes potential time-variant behavior due to temperature changes in the setup as well as the risk of harming the specimen during testing.

The experimental nonlinear modal analysis method is robust even in the presence of strong (damping) nonlinearities and sufficiently mature to be applied to industrial structures such as turbine blades. This is illustrated in the talk by means of specimen with a large range of nonlinearities. Moreover, the method's usefulness for other purposes such as characterizing and analyzing isolated frequency response branches is addressed. Furthermore, the benefit of higher harmonic excitation to counteract undesired exciter-structure interactions is discussed.

Modal Analysis and Modal Damping of MIKOTA's Vibration Chain

Müller, Peter C. (1); Weber, Wolfgang (2) 09:10
1: University of Wuppertal
2: Helmut Schmidt University, University of the Federal Armed Forces Hamburg

In [1] MIKOTA's vibration chain with a special mass matrix $M = M^T > 0$ and stiffness matrix $K = K^T > 0$ has been completely solved showing normalized eigenfrequencies $|w_j| = j$, where $j = 1, \ldots, n$ and a recursion formula for the eigenvectors z_j depending on power vectors $y_j = [1^j, 2^j, 3^j, \ldots, n^j]^T$. In the present contribution firstly a new calculation scheme for the eigenvectors z_j is presented using modified orthogonalized GRAM-SCHMIDT vectors based on the power vectors y_j. By this new method five eigenvectors are explicitly calculated as an example.
In a second part modal damping of the vibration chain is discussed, i.e. an additional damping term is included in the above-mentioned differential equation where $D = D^T > 0$ satisfies the condition

$DM^{(}-1)K = KM^{(}-1)D$. Designing D with respect to LEHR's damping measure and then for uniform measures, the modal damping matrix is determined. Therefore, the modal damping matrix can be calculated either by the eigenvalues and eigenvectors of the conservative system or by the given data of the mass and stiffness matrices without knowing the mode shapes.

Reference:
[1] P.C. Müller, W. E. Weber: Modal analysis and insights into damping phenomena of a special vibration chain. Arch Appl Mech 91, 2179–2187 (2021). https://doi.org/10.1007/s00419-020-01876-z.

Experimental analysis of oscillations of a rotor supported by gas foil bearings.

Sorgec, Berk; Liebich, Robert
TU Berlin

09:30

Gas foil bearings (GFB) are machine components that offer certain advantages for specific applications such as (micro-) turbomachinery, given adequate operation conditions, such as comparatively low load and high rotational speed. Advantages may include low wear and maintenance, low frictional losses, tolerance to extreme temperatures and absence of oil lubrication systems and the associated weight, complexity and possible contamination of process media (e.g., air in compressors for fuel cells). However, gas foil journal bearings (GFJB) are prone to exert self-excited non-linear vibrations, causing the supported rotor to oscillate with high amplitudes.

In this contribution, an experimental analysis of a rotor supported by two gas foil journal- and thrust bearings, respectively, is performed. The obtained signals are transformed into frequency domain and rigid body modes of the rotor (cylindrical and conical) are separated and analysed using amplitude- and phase spectra. Sub-synchronous whirl and whip phenomena are present and allow themselves to be assigned to a rigid body mode of the rotor.

Inductive mode selective damping of structural vibrations

Rosenboom, Mitja; Hetzler, Hartmut
University of Kassel

09:50

Structural vibrations pose significant challenges in various engineering applications and require effective damping strategies to improve the overall performance and longevity of systems. Thus, the reduction especially of resonance amplitudes is an important and recent field of research, which is underlined by the promotion of the DFG for the priority program "calm, smooth and smart", that this work is part of.

This contribution presents a novel method for damping of structural vibrations by selectively targeting specific modes, which can be beneficial in situations where a precise control of specific vibration modes is essential. For example, this approach can enhance energy efficiency by concentrating damping on critical resonances, preventing unnecessary dissipation across non-critical modes. Moreover, the preservation of desired modes may ensure that dynamic behaviors contributing positively to the system's overall performance remain largely unaffected, while critical modes are reduced effectively.

To achieve a mode selective damping behavior a passive approach is used within this work. It is based on multiple inductive damping elements distributed over a structure, that interconnect with each other electrically. The principle and the functionality are illustrated by means of a minimal model consisting of an oscillator chain with basic inductive damping elements. These consist of a permanent magnet moving inside of electrical coils.

The presentation begins by establishing the benefits of mode selective damping and giving a brief introduction of the design and calculation of the inductive damping elements. After presenting the investigated minimal model and displaying its dynamical behavior, a systematic study of the different

interconnections of the inductive damping elements is given. Thereby the different abilities of the considered approach are shown and discussed in detail.

S05.02: Oscillations (2)

Date: March 19, 2024 16:30–18:30
Room: G22/217
Chair(s): Stender, Merten

Friction damping in structural dynamics: from fundamental understanding to physics-based machine learning identification

Marino, Luca 16:30
TU Delft

Structural joints characterised by moving surfaces are present in most engineering structures. Identifying the nonlinear forces generated by frictional interfaces, as well as understanding how their damping effects can be exploited to achieve vibration reduction and energy dissipation, are among the present critical challenges in structural dynamics. Moreover, the unpredicted nonlinear behaviour induced by friction can lead to undesirable effects, such as stuck contacts, stick-slip, excessive oscillations and even unexpected failures. Predicting the nonlinear response of friction damped systems is therefore essential to develop robust designs and efficient monitoring strategies. Nonetheless, the analysis and identification of these systems is complicated by the nonlinear and nonsmooth nature of the frictional forces, which is responsible for the generating sharp variations and multiple motion regimes in their dynamic response.

This contribution deals with three major challenges: (i) the derivation of analytical solutions for the response of discrete mechanical systems with Coulomb friction, and the prediction of their motion regimes; (ii) the development of an experimental framework for reproducing and validating the proposed mathematical solutions; (iii) the formulation of a physics-based machine learning approach for the identification of frictional systems.

Mathematical solutions are obtained for the steady-state response of single- and multi-degree-of-freedom (DOF) systems with a friction contact to harmonic excitation. The derived formulations also enable the investigation of the dynamic behaviour of systems with oscillating contacting parts and/or different forms of damping. The results include the analytical prediction of the motion regimes (continuous, stick-slip, permanent sticking) and the displacement transmissibility curves resulting from varying system parameters.

The experimental investigation is performed on shear-frame setup with a brass-to-steel contact, able to reproduce the behaviour of single- and 2-DOF systems in contact with a fixed or oscillating wall. Tests run at different exciting frequencies and friction force amplitudes were able to closely reproduce the theoretical results, showing that Coulomb model can be used, in most conditions, for describing the dynamic behaviour of structures with a metal-to-metal contact.

The proposed identification method combines a partially-known physics-based model of the system with noisy measurements of its response in a switching Gaussian process (GP) latent force model, where multiple GPs are used to model the nonlinear force across different motion regimes and a resetting model to generate discontinuities. Regime transitions and discontinuities are inferred in a Bayesian manner, along with the nonlinear force, and can be used to implement forward models able to make reliable response predictions.

A Rational Ansatz for the Approximation of Koopman Eigenfunctions

Römer, Ulrich J.; Breitenhuber, Margarete 17:10
Karlsruhe Institute of Technology

Koopman operator theory as a basis for the systematic transformation and linearization of complex dynamical systems has attracted great interest in the dynamics community over the last decade and

a half. Given an autonomous nonlinear differential equation d**x**/dt=**f**(**x**) for the states **x**, any eigenfunction φ(**x**) of the associated Koopman operator (semi-)group and its generator have the dynamics dφ/dt = $\lambda\varphi$, where $\lambda$is the corresponding eigenvalue. We take the perspective that the (approximate) calculation of eigenfunctions of the Koopman operator (called Koopman eigenfunctions) as a systematic approach to transformation from the original states **x** to new coordinates φ with (decoupled) linear dynamics, which is an extension of modal analysis to nonlinear systems. If the original system is already linear d**x**/dt=**Ax**, the (principal) Koopman eigenfunctions ψ=**l***x —also known as modal coordinates in this case—are linear and can be calculated directly by the scalar products of the left-eigenvectors **l** of **A** with the state vector **x**.

While Koopman operator theory is often used as the basis for data driven methods, we assume that we already have some model d**x**/dt=**f**(**x**) for which we want to find a coordinate transformations φ(**x**) that linearize and decouple the system. The basis for our approach is an extension of the Hartman-Grobman theorem [1] that we crudely paraphrase as: the (principal) Koopman eigenfunctions φ in the basin of attraction of a (non-resonant) hyperbolic fixed point of a sufficiently smooth nonlinear system d**x**/dt=**f**(**x**) are the nonlinear extensions of the Koopman eigenfunctions ψ of the linearized system d**x**/dt=(∇**f**)**x** with the same eigenvalues λ.

To calculate approximations of Koopman eigenfunctions, we propose a rational ansatz φ(**x**)=n(**x**)/d(**x**), where the numerator is a linear combination n(**x**)=ξ_n*Θ(**x**) of m ansatz functions Θ(**x**)=[Θ_1(**x**),…,Θ_m(**x**)] with unknown coefficients ξ_n and the denominator is d(**x**)=ξ_d*Θ(**x**). The unknown coefficients ξ_n and ξ_d are determined from a constrained optimization problem in order to satisfy the extension of the Hartman-Grobman theorem while minimizing a suitably defined residual to (approximately) satisfy dφ/dt = $\lambda\varphi$.

We exemplify our approach with a damped pendulum with one (globally) stable fixed point and one unstable fixed point and compare it to a linear ansatz, i.e. to a classical Galerkin approach.

[1] Lan, Y.Mezić, I.: Linearization in the large of nonlinear systems and Koopman operator spectrum. Physica D: Nonlinear Phenomena 242(1), 42–53 (2013)

Quantifying Uncertainty in Neural Network predictions of forced vibrations

Westmeier, Tobias (1); Kreuter, Daniel (1); Hetzler, Hartmut (2); Seitz, Philipp (3); Chalvatzaki, Georgia (3)
1: Robert Bosch GmbH
2: University of Kassel
3: TU Darmstadt

17:30

Predicting the forced vibrations of nonlinear systems is a typical task in science and engineering. Common approaches are usually based on physical laws (" first principles"), which yield differential (algebraic) equations (ODEs, PDEs, DAEs) that have to be solved numerically. We bypass the classical derivation step and obtain models for nonlinear dynamical behaviour by various data-driven approaches. Here, we compare stabilised Autoregressive Neural Networks (s-ARNNs) to architectures with implemented memory (DeepAR) and transformer-based architectures and benchmark against linear methods. A fundamental limitation of Neural Networks is their lack of transparency, making it difficult to understand and trust the model's decisions.
We examine several approaches to quantify uncertainty in s-ARNNs. Our proposed approach combines Mean-Variance Estimation (MVE) to estimate the aleatoric uncertainty and Deep Ensembles to measure epistemic uncertainty. We demonstrate that our approach outperforms other methods like DeepAR and temporal fusion transformer and classical approaches with homoscedastic uncertainty. Our method excels in accuracy and uncertainty reliability on synthetic and real-world datasets, including a Duffing oscillator and a steering system. Our comparison establishes the MVE Ensemble as the most accurate and reliable method for uncertainty quantification, showing that it is advantageous to quantify both aleatoric and epistemic uncertainty. Our findings demonstrate the significance of understanding uncertainties in deep neural networks and the relevance of our method in improving the reliability of predictions in nonlinear systems under dynamic load.

Complex dynamics of coupled nonlinear oscillators from a functional networks perspective

Geier, Charlotte (1); Stender, Merten (2); Hoffmann, Norbert (1,3) 17:50
1: Hamburg University of Technology
2: TU Berlin
3: Imperial College London

Network methods are well established in many areas of science, such as medicine or climate research, and provide a range of approaches to studying oscillating dynamical systems. This work uses network-based measures to introduce a functional network perspective on the dynamics of mechanical multi-component systems. Despite an extensive available toolset, some aspects of the dynamics of these engineering systems remain difficult to understand even today. Phenomena such as nonlinearities pose challenges to state-of-the-art system identification and modeling approaches. These nonlinearities arise from large deformations, joints, friction, or material properties, and are especially difficult to handle in large, multi-component systems. At the same time, the dynamics of these large machines need to be better understood to ensure adequate design and safe operation, including avoiding potentially harmful oscillations.

Our work seeks to complement classical time- or frequency-domain-based methods for analyzing and describing the dynamics of complex mechanical multi-component systems with a novel, function-based perspective. In our functional network, each node represents a component of the mechanical model system, and the edges between the nodes denote functional relationships between two components. This functional relationship is established based on specific recurrence network measures, which are computed from time series measurements from the components. These measures describe the dynamical inter-dependency between two components. Thus, the functional network represents functional relationships in the mechanical system rather than the geometrical proximity of the components.

This complementary perspective on the dynamics of complex mechanical systems opens the door to new network-based methods. For example, our functional networks help uncover the dimensionality of the phase space of the underlying dynamical system from data, reveal functional dependencies within a mechanical multi-component system, and enable the tracking of disturbance propagation through a system. These findings pave the way to new approaches in model-order reduction, suitable sensor placement, and countermeasures (in design or during operation) against unwanted and potentially harmful vibrations.

Characterization of music effect pedals by data analysis

Rentzsch, Frederik; Wulff, Paul; Gödecker, Holger; von Wagner, Utz 18:10
TU Berlin

Effect pedals are used to obtain a distorted sound by manipulating the voltage signal of an instrument, e.g. an electric guitar. In recent times, the modelling of this dynamic transmission behavior has been of great interest, as it allows certain sound settings of one or more effect pedals in the signal chain to be stored and loaded digitally. Novel machine learning techniques make it possible to generate very accurate models without prior knowledge of the system. On the other hand, there are regression methods, like Sparse Identification of Nonlinear Dynamics (SINDy) that are used to reduce large models to a significant size.

In the actual presentation, a method is proposed that combines both aforementioned approaches. Firstly, a randomly initialized neural network of type Reservoir Computer is generated. Secondly, the network is reduced to a small size by cancelling out irrelevant linear parameters using SINDy. Lastly,

remaining nonlinear network parameters of the reduced model are optimized. Based on experimental data of measurements with a guitar effect, it is shown that this approach leads to small and at the same time precise models, as they are desired for the application under consideration.

S05.03: Oscillations (3)

Date: March 20, 2024 14:00–16:00
Room: G22/217
Chair(s): Stender, Merten

Numerical detection of suppression of quasi-periodic solutions

Seifert, Alexander; Hetzler, Hartmut 14:00
University of Kassel

In science and technology, the investigation of dynamical systems plays a key role. A dynamical system can show different types of stationary solutions (e.g. equilibrium, periodic, chaotic). In recent years the focus of academic research shifted towards quasi-periodic solutions. These solutions retain a discrete frequency spectrum, which can be expressed by a linear combination of so-called base frequencies, which are incommensurable. Although the frequency spectrum is discrete the solution does not show periodic behaviour. Due to the fact, that the solution is composed of a finite number of base frequencies, it can be represented by a toroidal manifold of the same dimension. The ergodic theorem allows to calculate the manifold instead of the time solution, due to the fact that the quasi-periodic motion itself is ergodic. To calculate the manifold in a systematic way, one can use the hyper-time parametrization. The manifold can then be calculated by solving a partial differential equation over a finite set. The main disadvantage of this parametrization is, that it is only valid as long as the number of base frequencies is unchanged.

If a quasi-periodic solution branch is continued, the solution can show the phenomenon of synchronization, in which the number of base frequencies is reduced. This poses a problem, when using the hyper-time parametrization, due to the fact that it is no longer valid in case of synchronization. It is therefore crucial to detect an approach to a synchronization point. There exists no bifurcation theory for quasi-periodic solutions yet. There are multiple ways a solution may synchronize. We will focus on the detection of the suppression of the natural dynamics (i.e. the detection of a Neimark-Sacker bifurcation).

The detection of Neimark-Sacker bifurcations by a test function based on the quasi-periodic solution is not possible, due to the fact that the hyper-time parametrization is utilized and we therefore cannot continue the solution branch through the bifurcation point. Thus, we cannot achieve a strict root in a test function.

Instead we want to detect an approach to the bifurcation. This can be done by analysing the hyper-time manifold itself. We will show an approach which is based on the arclength of sections of the hyper-time manifold and derive a, in general, non-square matrix. We can then detect a Neimark-Sacker bifurcation based on its singular values. We will show that our approach can also be used to detect quenching (i.e. codim-2 bifurcations).

SBFEM with perturbation method for solving the Reynolds equation

Pfeil, Simon (1); Song, Chongmin (2); Woschke, Elmar (1) 14:20
1: Otto von Guericke University Magdeburg
2: University of New South Wales, Australia

Rotordynamic simulations with nonlinear hydrodynamic bearing forces require a solution of the Reynolds equation at every time step. As a computationally efficient alternative to the standard numerical methods, a semi-analytical solution based on the scaled boundary finite element method (SBFEM) was developed recently. Through a discretization of the hydrodynamic pressure (dependent variable) along the circumferential but not the axial coordinate, the partial differential equation is transformed into a system of ordinary differential equations. This system of differential equations is referred to as SBFEM equation and can be solved exactly if the influence of shaft tilting is neglected.

In common numerical models, this influence can be taken into account without difficulties, but as far as this semi-analytical approach is concerned, shaft tilting complicates the equations substantially. Therefore, previous studies on the SBFEM solution of the Reynolds equation were conducted without consideration of this effect. The formulation presented in the work at hand no longer requires this simplification. The terms representing the influence of shaft tilting in the SBFEM equation are handled by the perturbation method. The pressure field is expressed by a series expansion, where the solution of order k correlates to the k-th power of a perturbation parameter chosen proportional to the tilting angle. The differential equation governing the k-th solution contains lower-order solutions on its right-hand side, implying a recursive computation of the series from lowest to highest order. A universal expression for the general solution is formulated, where only the coefficients and the maximum power of the axial coordinate differ for every k. This allows the implementation of a general algorithm with no inherent limitation regarding the maximum order of perturbation. For verification, the pressure fields computed by the proposed method are compared to a numerical reference solution, showing that the series converges to the correct result for the investigated set of parameters.

Shape optimization for MEMS gyroscopes

Schiwietz, Daniel; Hörsting, Marian; Degenfeld-Schonburg, Peter; Wenzel, Matthias
Robert Bosch GmbH

14:40

Requirements regarding noise and zero-rate offset-values for micro-electromechanical gyroscopes for consumer and automotive applications are steadily increasing. Unexpected system failures often originate from nonlinear coupled oscillations of the driven mode with parasitic modes. Circumventing these errors is a challenging task for state-of-the-art design tools.
In this work, we develop a gradient based shape optimization scheme to control nonlinear mode couplings of micro-electromechanical gyroscopes and thus can improve zero-rate offset performance. The gyroscopes main features, e.g., the natural frequency of the driven and sense mode as well as manufacturing constraints are adhered to by employing additional constraints in the objective function. To ensure an efficient implementation, the objective function gradients are derived manually and solved for using an adjoint analysis. The presented scheme is not only applicable to micro-electromechanical systems but may in the future be applied to vibrating systems in general.

Modeling of oscillating piezoelectric actuators with cracks

Riedel, Simon (1); Kapelke, Simon (1); Fidlin, Alexander (2)
1: Physik Instrumente (PI) GmbH & Co. KG
2: Karlsruhe Institute of Technology

15:00

Piezoelectric actuators, which are commonly used to drive high-precision positioning systems, can withstand very high compressive loads, but are sensitive to tensile stresses. Cyclic loads and frequent load changes as well as incorrect mounting can cause mechanical failures such as cracks, in particular when the piezoelectric actuator is of multilayer type. The influence of these cracks on the electromechanical behavior and the durability of the piezoelectric actuator is the subject of current research. The aim is to clarify if a prediction of failure or remaining lifetime is possible based on the dynamic behavior of the actuator.

Changes in the natural frequencies or the dynamic behavior in general could indicate cracks in the piezoelectric actuator. For this reason, models are needed that can reproduce the dynamic behavior of the actuator properly. Mechanical models, electro-mechanical models and electrical equivalent circuits are being investigated for this purpose. Furthermore, the impact of cracks on the behavior in normal operation, i.e. at low operating frequencies, as well as on the lifetime of the piezoelectric actuator are of interest.

S06.1: Material modelling with metals

Organizer(s): Mosler, Jörn *(TU Dortmund University)*
Kurzeja, Patrick *(TU Dortmund University)*

S06.1.01: Various topics in Material modelling with metals

Date: March 20, 2024 08:30–09:30
Room: G16/H5
Chair(s): Kurzeja, Patrick
Mosler, Jörn

Merging traditional and neural network material modeling

Meyer, Knut Andreas
TU Braunschweig

08:30

For over a century, researchers have refined plasticity models motivated by material microstructure, physical constraints, and experimental data. On the other hand, recent hardware and software advancements have made deep neural networks increasingly viable for material modeling. This talk will focus on challenges in plasticity modeling and how combining traditional and machine-learning modeling approaches can overcome these challenges.

The yield surface evolution caused by large shear strains, experimentally investigated in [1], poses a challenging material modeling problem. Specifically, initial softening followed by hardening could be observed, along with yield surface distortion. Describing such behavior consistently for finite strains required novel model formulations and calibration strategies [2]. Moreover, during that work, we discovered how most plasticity models share one crucial assumption for isotropic and distortional hardening; they only depend on the accumulated plasticity for some loading cases. This discovery prompted an investigation of this assumption, showing that it did not hold for the investigated steel [3]. In conclusion, this implies that traditional models cannot correctly describe hardening for this standard material.

After identifying this shortcoming of existing models, the natural question is how to solve this: Specifically, can data-driven approaches overcome the limitations of current models? In response, a novel approach for combining neural networks and traditional material modeling was developed [4]. The first unique feature of that approach is the ability to fulfill thermodynamic requirements, even without training. Furthermore, the neural network-enhanced plasticity model could, in contrast to existing models, describe the behavior seen in [3]. The second unique feature of the approach in [4] is the ability to discover analytical and interpretable material models – removing the black-box neural network modeling components.

Despite successfully capturing the isotropic hardening behavior, the model in [4] could not perfectly fit the experimental results. To improve this situation, the last part of this talk will focus on a novel plasticity model having a smooth elastic-to-plastic transition. In particular, these advances highlight the necessity of pushing research boundaries of traditional material modeling and data-driven approaches in synergy.

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On neural networks as propagators in data-driven inelasticity

Harnisch, Marius (1); Bartel, Thorsten (1); Schweizer, Ben (2); Menzel, Andreas (1,3)

1: Institute of Mechanics, TU Dortmund University
2: Chair I (Analysis), TU Dortmund University
3: Division of Solid Mechanics, Lund University

09:10

Data-driven mechanics, introduced by Kirchdoerfer and Ortiz [1], replaces conventional material modeling with data-sets containing snapshots of stress and strain assumed to be sufficiently accurate representations of the underlying material behavior. Build on these snapshots, termed material states, and on states fulfilling equilibrium and kinematic compatibility, called mechanical states, is a distance function, whose minimization with respect to both the material and mechanical states yields the boundary value problems' solution.

Originally introduced for elasticity, an extension to inelasticity poses a significant challenge for the scientific community and besides our extension [2], different approaches have been proposed. However, by building our novel extension on a quantity called history surrogate and an accompying propagator, we preserve the spirit of the original approach and dispense the need of on-the-fly data-set adjustments. The history surrogate thereby stores essential information of the history of the material up to the current point in time and the propagator serves as an update rule at the end of each time step. This allows for an offline definition of our synthetic data-set which remains fixed during online data-driven simulations. The challenge now shifts to defining a history surrogate both suitable and generally applicable - a complex task if tackled by hand. We therefore advocate a framework utilizing a Neural Network as propagator, which autonomously extracts the essential information of the materials history without resorting to a material model. Such a model is solely required when generating the raw input data in form of discrete paths. From there on, the neural network propagator allows for an automated framework, ranging from the construction of the data-set with a suitable history surrogate to the solution of boundary value problems with inelastic material behavior.

In this contribution, we introduce our extension to inelasticity and highlight the capabilities of our novel approach. By presenting results for different inelastic processes utilizing a neural network progagator, we focus on the resulting automated framework which such neural network allows for. We show the necessary training routines of the network, discuss the obtained data-driven simulations and provide a comparison with an intuitive choice of history surrogate and propagator.

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S06.1.02: Various topics in Material modelling with metals

Date: March 20, 2024 14:00–16:00
Room: G16/H5
Chair(s): Kurzeja, Patrick
Mosler, Jörn

Damage-Plasticity Models at Finite Strains: Gradient-Enhancements, Calibration and Numerics

Friedlein, Johannes; Steinmann, Paul; Mergheim, Julia

FAU Erlangen-Nürnberg

14:00

Material modelling for the simulation of clinching processes involves large plastic strains which are inherently linked to the evolution of damage. This (plasticity-driven) ductile damage can affect manufacturing processes and product lifetimes. The modelling and identification of the process-induced damage is here conducted by means of a fully coupled plasticity-damage continuum material model at finite strains. We compare different approaches for gradient-enhancement to regularise the coupled

problem, including “plasticity - gradient-damage”, where the gradient-enhancement is applied to the damage variable, and “gradient-plasticity - damage” with a gradient-enhanced plasticity formulation.

The application of the material models to simulate clinching processes requires their calibration for particular materials, here for an aluminium alloy and a dual-phase steel. First, the experimental parameter identification for anisotropic plasticity models and their validation are shown. The calibrated models are then used within a clinching simulation to identify the influence of the anisotropy on the clinching process and the resulting geometry of the clinch point. Further attention is paid to the identification of the internal length associated with gradient-enhanced models. The choice of the variable, that is regularized, does not only affect 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, such that e.g. a directly identified failure strain is not accurately reproduced. This can complicate inverse parameter identifications, especially when many experiments need to be considered simultaneously as for coupled stress-state dependent damage models.

Finally, 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 become evident in the conducted parameter identification for sheet metal.

Quantification of the effect of uncertainty of material parameters on damage initiation in finite strain elastoplasticity

Böddecker, Merlin (1); Faes, Matthias Gustaaf Rene (2); Menzel, Andreas (1,3); Valdebenito, Marcos Alberto (2)

1: Institute of Mechanics, TU Dortmund University
2: Chair for Reliability Engineering, TU Dortmund University
3: Lund University

14:40

In metal forming processes, initial material properties, among other factors, influence the component’s life time and performance properties together with deformation induced material degradation. In process simulations, initial material properties, such as material parameters, are typically assumed to be constant for a given material, i.e. constant across different material batches. In practise, however, initial material properties exhibit uncertainty due to intrinsic variabilities resulting from, e.g., casting and preceding production processes. To enhance metal forming process simulations with regard to variability in resulting material parameters, quantifying such uncertainty is most important for reliable simulation-based prediction of process-induced material properties.

To this end, a numerically efficient variance-based global sensitivity analysis framework is developed [1] to quantify the effect of uncertainty of material parameters on damage initiation indicators, such as stress triaxiality and Lode angle. The established framework incorporates a Gaussian regression surrogate model along with a Bayesian active learning strategy to improve the computational efficiency. A key challenge in its application to the boundary value problem of a tensile test specimen are localisation effects of plastic contributions and resulting mesh-dependency observed beyond the onset of necking, preventing further uncertainty quantification. To overcome such localisation, a micromorphic- and gradient-type regularisation for plasticity is implemented, which enables uncertainty quantification at high loadings. Its application reveals that extremal values of damage initiation indicators show particularly high sensitivity for parameters related to nonlinear hardening and underlines the potential of damage control through optimisation of the material’s nonlinear hardening behaviour.

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Modeling and identifying yield stress and Taylor-Quinney factor using a thermodynamic consistent constitutive theory and infrared thermography measurements

Lalovic, Nikola; Dyck, Alexander; Kauffmann, Alexander; Heilmaier, Martin; Böhlke, Thomas 15:00
Karlsruhe Institute of Technology

Classically, a phenomenological approach (i.e., a constant Taylor-Quinney factor) is chosen to predict self-heating of metals. However, this approach does not fulfill basic thermodynamic principles [1,2]. In this talk, a thermodynamically consistent expression for the self-heating of thermo-elasto-plastic metals is derived in a small deformation setting with an isotropic, rate-independent von Mises plasticity theory. Based on the proposed framework, the internal dissipation and the fraction of plastic work converted to heat (i.e., the Taylor-Quinney factor) is studied in detail. It is shown, that within this framework the yield stress is additively composed of an energetic and a thermal part, which allows to predict self-heating and stored energy of cold work during plastic deformation of metals. The proposed model is identified by using infrared thermography measurements [3] conducted during uniaxial tensile tests on aluminium specimens.

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An experimental and numerical benchmark: Evolution of forming induced residual stresses under cyclic loading

Schneider, Tom; Kästner, Markus 15:20
TU Dresden

Under cyclic loading, residual stresses can significantly affect a metallic component's performance. Engineering structure design and manufacturing processes may be improved by having a better understanding of the amount, occurrence, and behavior of residual stresses under such loading. In particular, when it comes to extending fatigue life, compressive residual stresses are very advantageous. This is only true, though, if the residual stresses remain in the structure for the whole fatigue life. For this reason, it is important to examine how residual stresses change during cyclic loading.
An experimental setup to investigate the formation and cyclic evolution of forming induced residual stresses is given in the talk. Simulations are used in conjunction with the tests to highlight pertinent problems with modeling residual stress evolution under cyclic loading. Four-point bending specimens are utilized since they enable a pure bending state which is one of the simplest inhomogeneous loading situations required for residual stress formation. Following the initial loading, they experience cyclic deformation, which modifies the residual stresses relative to the initial state. The experiment is terminated at different load cycles during the fatigue life, and the specimens are used to measure the residual stress condition experimentally using the incremental hole drilling method. Next, a comparison is made between the simulation and the experimental results on the evolution of the cyclic residual stress. The implementation and parameterization of a plasticity model that can capture the effects of cyclic plasticity are demonstrated and contrasted with experimental data gathered from the cyclic bending tests. It is shown that modeling the evolution of residual stress is a challenging task whose results must be carefully evaluated regarding the model definition and parameterization.

Modelling cyclic behavior of high-temperature steels: a two-time-scale approach

Knape, Katharina; Altenbach, Holm; Naumenko, Konstantin 15:40
Otto von Guericke University Magdeburg

Nowadays, gas turbines generate a significant amount of electricity especially in order to close the gap caused by the unpredictable output of the renewable resources. This running mode implies various start-ups and shut-downs of the system as well as enormous load changes subjecting the components not only to high temperature conditions but also cyclic loads in the form of periodic stress

and strain states. The combination of both, mechanical and thermal demands, greatly influences the component's life and may lead to failure earlier than expected. To prevent unforeseen events and investment costs, an understanding of the material's behavior and response through a reliable simulation is mandatory.

An advanced constitutive model with hardening and softening rules, including a constitutive equation for the inelastic strain rate and an evolution equation for the backstress tensor is considered as basis for modelling the material behavior of high-temperature steels. Since a cycle-by-cycle simulation usually becomes numerically expensive due to very small time increments, the two-time-scale approach is implemented to reduce the computational time. It considers a slow time scale, also referred to as the physical time and accounting for long-term processes as well as a fast time scale describing the cyclic behavior. The overall aim is to achieve a decoupled system of differential equations using an asymptotic series expansion in order to solve them separately.

The finite element software ABAQUS is used, including a user material subroutine in combination with a python script to carry out the solving algorithm of the two time scales.

S06.1.03: Various topics in Material modelling with metals

Date: March 21, 2024 14:00–16:00
Room: G16/H5
Chair(s): Mosler, Jörn
Kurzeja, Patrick

An efficient implementation of a micromorphic gradient extended, rate-independent single crystal plasticity model based on an Augmented Lagrangian formulation

Prüger, Stefan; Kiefer, Bjoern 14:00
TU Bergakademie Freiberg

A size-dependent mechanical response of metallic, crystalline materials is observed, if the characteristic dimensions of structural components are of the same order as the characteristic dimensions of the microstructure, e.g. the grain size. Experimental evidence of this phenomenon is typically found in wire torsion, thin-film bending, micropillar compression and micro indentation experiments. As local constitutive models are not capable to reproduce these size effects, local material models are generally extended by means of a set of additional field variables, which have to satisfy additional boundary value problems. The latter can be derived for example from the extended principle of virtual power.
In the current contribution, the reduced micromorphic gradient crystal plasticity model, introduced in [C. Ling, et al., Int. J. Solids Struct., 2018, 134:43-69], is adopted and implemented in a rate-independent format based on an Augmented Lagrangian formulation of the principle of maximum dissipation [S. Prüger, B. Kiefer, Int. J. Mech. Sci.,2020, 180:105740]. In particular, the implementation into the finite element code Abaqus is presented, which exploits the analogy between the balance relation for the micromorphic counterpart of the accumulated equivalent plastic strain and the stationary heat equation. The robustness and the capability of the model to predict size-dependent material response is assessed by means of representative, three-dimensional finite element simulations of wire torsion and bending.

Barrier parameter update strategies for interior-point methods in single crystal plasticity

Steinmetz, Felix; Scheunemann, Lisa 14:20
RPTU Kaiserslautern-Landau

Simulating the deformation behavior of crystals helps in gaining insights into the behavior of polycrystalline materials like metals and alloys. Single crystal plasticity seeks to simulate the mechanical behavior of a single crystalline grain derived from its crystallographic structure. This approach is expressed mathematically using the concept of multisurface plasticity. By applying the principle of maximum plastic dissipation, an optimization problem emerges, wherein the crystal's slip systems, determine the constraints.

Within the context of rate-independent crystal plasticity models, the set of active slip systems may not be unique, posing a challenge to its algorithmic treatment. Conventional strategies involve an active set search incorporating diverse regularization techniques [3] or problem simplifications to achieve uniqueness [1]. Given the need for multiple evaluations in computationally extensive simulations, a stable, robust, and efficient algorithm is needed.

Recently, a new approach utilizing the infeasible primal-dual interior point method (IPDIPM) [2] has been introduced in [4]. This method addresses the ill-posed problem without relying on perturbation techniques. In the IPDIPM, barrier functions are used to penalize infeasible solutions. However, in contrast to classical penalty methods, this penalization is implemented in a smooth way and gradually increases when the limit of the feasible domain is reached. It involves the so-called barrier parameter, which approaches zero gradually, creating a sequence of optimization problems to be solved. This is typically done within a sequence of Newton schemes, wherein the modification of the barrier parameter has great influence on the performance and stability. This talk especially focuses on the treatment of the barrier parameter, addresses pertinent numerical aspects of the algorithm, and explores effects on the algorithm's performance and convergence.

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On discrete conservation of constraints in microstructure evolution

Bode, Tobias; Soleimani, Meisam; Erdogan, Cem; Wriggers, Peter; Junker, Philipp 14:40
Leibniz University Hannover

In materials science, microstructure evolution plays a central role in understanding and predicting the behavior of materials under different conditions. The development of the microstructure is often subject to certain constraints. A classic example of such a constraint is volume conservation during plastic deformation in the context of elasto-plasticity.
Within the talk, two principles are compared for the imposition of constraints in evolution equations: the principle of maximum dissipation with respect to the stresses and the principle of the minimum of the dissipation potential with respect to the rate of thermodynamic state variables, which can be derived from a Hamiltonean principle. These principles serve as a basis for the formulation of material models that describe the internal structure and the reaction of materials to external influences. The principle of maximum dissipation provides the most energetically unfavorable form of stress distribution, while the principle of minimum dissipation seeks the most energetically efficient rate of change of the state variables.
In general, a discretization has to be applied for the numerical implementation of material models. Frequently, the discretization does not pay sufficient attention to the exact fulfillment of the constraints, which can severely limit the robustness and accuracy of the resulting model. Discretizations that guarantee compliance with the constraints, such as the exponential map, are often complex and challenging to implement. However, the principle of minimum dissipation illustrates that it is generally possible to fulfill constraints precisely with more simple time derivatives via the method of Lagrange multipliers. Using the example of finite elasto-plasticity, a volume-preserving time integration method based on backward Euler is presented.

On the adaptive solution of phase-field problems with A-stable explicit last-stage diagonally implicit Runge-Kutta (ELDIRK) methods

Westermann, Hendrik; Mahnken, Rolf
Paderborn University

15:00

Runge-Kutta algorithms with adaptive step size control provide reliable tools for the solution of initial value problems with diagonally implicit Runge-Kutta (DIRK) methods as the most common approach. In particular, the new low-order explicit last-stage diagonally implicit Runge-Kutta (ELDIRK) methods are investigated, combining implicit schemes with an additional explicit evaluation as an explicit last stage. This results in Butcher tableaus with two solutions of different convergence orders suitable for embedded methods, where the higher-order solution is achieved by additional explicit evaluations. Thus, the iterative solution of non-linear systems is omitted for the additional stage, presenting a major reduction in computational cost for the determination of a local error estimate. The key contribution is the application of the novel Butcher tableaux to phase-field problems, solved with the finite-element method, leading to substantial numerical investigations with an efficient approach for diagonally implicit Runge-Kutta schemes. The most important aspects are the extension towards fourth-order methods and the substantial investigations of stability properties which lead to the novel class of A-stable ELDIRK methods. In accordance, the study of the convergence orders, and computational efficiency are presented. A local error estimator is presented capturing the evolution of the phase-field problems, such that adaptive step size control for the new low-order embedded schemes based on an empirical approach for error estimation is achieved. A suitable parallel algorithm is presented with conclusive two-dimensional phase-field simulations based on a Kobayashi-Warren-Carter model including benchmarks for computational efficiency. The higher-order convergence suggested by the novel schemes is confirmed, and their effective results are demonstrated, resulting in a valuable semi-explicit addition to the family of Runge-Kutta time integration schemes.

Latent heat in a thermomechanical theory for inclusion growth prediction via the multiphase-field method

Prahs, Andreas (1); Reder, Martin (2); Schneider, Daniel (1,2); Nestler, Britta (1,2)
1: Karlsruhe Institute of Technology
2: Karlsruhe University of Applied Sciences

15:20

In computational materials science, EBSD and μ-CT scans are key in the early stages of material characterization. However, designing a material to meet specific demands requires a considerable amount of scans, requesting significant personal and economic resources. The implementation of digital microstructures as a digital twin presents a more resourceefficient option. These microstructures, designed to emulate the properties of the scanned samples, are acquired through microstructure simulations. In this context, it is pivot that the digital microstructures provide a quantitative representation of the scanned microstructure. Consequently, the material model used as foundation for the numerical simulation of microstructure evolution must be as quantitative as possible. Modeling and simulation of the evolution of a complex microstructure with multiple phases is usually subject to the multiphase-field method [1], providing a numerically highly efficient treatment of moving interfaces [2]. However, even for non-isothermal phase transformations, the thermomechanical coupling is commonly neglected. Current studies [3] imply that this assumption is not justified, even for small strains and strain rates, if a non-vanishing coefficient of thermal expansion is considered. There, the plastic stress power and thermomechanical couple terms are considered as heat sources or sinks, respectively, regarding phase transformations involving plastification. In the current talk, the role of the latent heat, cf. [4], supplementing the framework of [3], is discussed with respect to displacive phase-transformations. Thereby, the growth of an elastoplastic inclusion, embedded in an elastoplastic matrix, under external loading, and subject to eigenstrains is discussed.

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S06.1.04: Various topics in Material modelling with metals

Date: March 21, 2024 17:40–18:40
Room: G16/H5
Chair(s): Prüger, Stefan
Mosler, Jörn

Modeling of the phase transformation behavior in metastable austentic stainless steels

Thammineni, Hari Kisan (1); Denzer, Ralf (2); Müller, Ralf (1) 17:40
1: TU Darmstadt
2: Lund University

The phenomenon of strain induced transformation to martensite in metastable austenitic steels is simulated using a phenomenological material model. It consists of a part that models kinetics of the austenite to martensite transformation; this is then coupled with a constitutive model that describes the stress-strain behavior in the resulting austenite–martensite composite. The constitutive model is based on hypo-elastoviscoplastic formulations, where the evolution of plastic strain in individual phases is modelled using viscoplastic flow equations. The hardening of the phases is also considered during the evolution of the plastic strains. The model is implemented as a material routine in a user element in FEAP using finite strain formulations. The rate equations are integrated with the backward Euler implicit time integration scheme. The parameters of the model are identified using experimental data of uniaxial tension tests and finally, the model is tested in illustrative boundary value problems.

Elasticity in phase-field crystal models of solidification

Punke, Maik; Salvalaglio, Marco 18:00
TU Dresden

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 [1,2,3]. 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 a recent extension of the classical PFC model: the coupling with a macroscopic velocity field, explicitly accounting for the relaxation of elastic excitations [4]. We examine how this model extension influences short- and long range behaviour of the elastic field.

Additionally, we apply our findings to novel aspects which were never touched before within the PFC framework, e.g. disconnections in two or three-dimensional elastic materials. We compare our results to molecular dynamics (MD) simulations and show, that the PFC accurately predicts short- and long range behaviour of the elastic field.

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Micromechanical multi-scale simulation of the directionally-solidified Mo-Hf-B alloy

Nizinkovskyi, Rostyslav; Naumenko, Konstantin; Krüger, Manja 18:20
Otto von Guericke University Magdeburg

Mo-based alloys are a feasible alternative to the current high-temperature materials for aerospace and energy industry applications due to high melting temperatures and exceptional creep resistance. Usage of Boron and Hafnium to build strengthening phases can improve creep resistance even further. In our work, we develop a methodology for study of micromechanics of near-eutectic directional solidified Mo-Hf-B alloy, containing ductile solid-solution and creep resistant intermetallic phases. The stochastic stereometric reconstruction technique based on combination of analytic solutions and Monte-Carlo method is revealed as well as stochastic microstructure generation. The micromechanical origins of eutectics anisotropy are revealed based on single lamellar RVE and analytic solutions. The phenomenological creep model for eutectic phase is described based on the aforementioned data. The steady-state creep response as function of microstructural characteristics is presented.

S06.2: Material modelling with non-metals

Organizer(s): Lion, Alexander *(Universität der Bundeswehr München)*
Kehrer, Loredana *(Karlsruhe Institute of Technology (KIT))*

S06.2.01: Various topics in Material modelling with non-metals

Date: March 19, 2024 08:30–10:30
Room: G16/H5
Chair(s): Kehrer, Loredana
Lion, Alexander

Multistage parameter identification of a finite-strain viscoelastic-viscoplastic material model for biobased thermosets

Laubert, Lukas; Pfaller, Sebastian 08:30
FAU Erlangen-Nürnberg

The modeling of intricate material behavior often requires complex constitutive models comprising a high number of parameters. In the course of reproducing the material response in creep recovery experiments via FE simulations of the biobased epoxy RE/DA-LIM derived from resorcinol diglycidyl ether (RE) and the hardener diamine-limonene (DA-LIM), we demonstrate a multistage procedure to separately calibrate parameters related to the elastic, viscoelastic, and viscoplastic domain, respectively, of a sophisticated viscoelastic-viscoplastic (VEVP) model. This model connects a hyperelastic bi-logarithmic elastic potential with quadratic dissipation in Maxwell branches to a viscoplastic formulation capable of capturing compression-tension flow asymmetry as well as isotropic and kinematic hardening. Each of these features encompasses multiple parameters, totaling 50 for the entire model. For calibrating those corresponding to the viscoelastic regime in a first step, we fit DMTA-TTS derived storage and loss modulus data, respectively. Subsequently, an inverse parameter identification is conducted by employing global optimization techniques for identifying the parameters related to the viscoplastic and elastic domain. To this end, data from several experimental setups is considered simultaneously by using an appropriate error measure. This approach represents a promising step in modeling the complex material behavior of biobased thermosets.

Frequency domain analysis of viscoelastic elastomer blends considering interfacial transition zones

Ulrich, Marc; Petö, Márton; Eisenträger, Sascha; Juhre, Daniel 08:50
Otto von Guericke University Magdeburg

In the field of elastomer technology, elastomer blends are widely utilized. In this study, the focus is on blends consisting of natural rubber and styrene-butadiene, with a volume fraction of 50%. Blends of these materials are especially prevalent in tire manufacturing. Within the examined mixture, there exists an interphase alongside the pure phases. Naturally, the polymer chains of each material solely exist in a pure phase. In between, there is an overlap at the phase transition between natural rubber and styrene-butadiene polymer chains. Describing and characterizing this viscoelastic material behavior requires considering the interphase. Since there is no secure knowledge concerning the properties of the interphase region, applying a pragmatic approach employing image processing techniques is well justified.

The use of a phase parameter allows for the description of the elastomer blend, wherein the parameter can take values between 0 and 1. Values of 0 and 1 indicate the pure material phases, while values in between represent a diffuse interphase. Previous methods for morphology analysis employed the Allen-Cahn equation to capture the multi-phase structure of the blend. However, this approach encountered computational time issues, since every morphology with varying interphase widths had to be calculated from scratch. The main advantage of the novel techniques lies in its computational efficiency compared to solving the Allen-Cahn equation.

In describing the viscoelastic material behavior, the characteristic properties of storage modulus and loss modulus are of greater significance. These describe the portion of energy stored in the material as deformation energy and the portion of energy dissipated as heat due to internal friction or dissipation when the material is stressed.

To this end a representative section of the microstructure, obtained from atomic force microscopy (AFM) is processed to determine the phase parameter. From this, the storage and loss moduli are calculated with spatial dependence across the microstructure. Elastomers exhibit frequency-dependent properties, thus analyzing the frequency dependence of these moduli is crucial. Different morphologies, based on the standard deviation of the Gaussian filter, allow for variation in the interphase. Three such morphologies with standard deviations σ= 5, 10, 15 were considered, and the frequency-dependent storage and loss moduli were calculated. Additionally, a finite element analysis was conducted to examine the different morphologies under shear loading.

This comprehensive investigation presents an alternative methodology for describing the complex structure-property relationship of elastomer blends, particularly concerning their interphase and its effects on viscoelastic behavior under various conditions.

Experimental analysis of a beam with a 2D triangular substructure

Panjalipoursangari, Narges; Morozov, Aleksandr; Müller, Wolfgang.H.; Völlmecke, Christina 09:10
TU Berlin

This study aims to experimentally determine the higher material parameter g of a metamaterial with a triangular substructure and validate a higher gradient elasticity model for beams with internal sub- or microstructures. Previous investigations into higher gradient elasticity models of Bernoulli-Euler and Timoshenko beams with periodic triangular substructure have demonstrated that the flexural stiffness is highly dependent on the geometric parameters of the lattice structure. The experimental approach involves the additive manufacturing of beams with triangular substructures using Fused Deposition Modeling and Stereolithography. These beams were subsequently subjected to tensile and bending tests. Three variations of beams with different numbers of layers (one, two, and four layers) of triangular structures were manufactured, utilizing two different materials, namely Polylactic Acid (PLA) and epoxy resin. The higher material parameter g was quantitatively determined based on the experimental results using an inverse analysis. In addition to the primary objective, this study investigates the relationship between flexural stiffness and the geometric parameters of the lattice structure. Another focus is on examining the influence of curing time on the elastic properties of epoxy resin. The experiments encompassed tensile and bending tests on the triangular beams, with numerical and experimental results compared using digital image correlation. Based on the experimental data, a higher gradient material parameter representing the geometric structure of the lattice was identified. Overall, this study significantly contributes to the current understanding of metamaterials and higher gradient elasticity models for beams with internal sub- or microstructures. The quantitative results provide a foundation for further refinement of numerical models and design guidelines for metamaterials. Additionally, future studies will extend the investigation to encompass a comprehensive mechanical characterization of innovative composite materials that combine biopolymer reinforcement with mushroom-based components. This endeavor aims to gain a thorough understanding of their mechanical performance and assess the potential applications of these novel materials across various industries.

Material Plasticity - Development of the material stiffness in fiber-reinforced materials with large plastic deformations

Weber, Martin; Glüge, Rainer; Altenbach, Holm 09:30
Otto von Guericke University Magdeburg

The objective of this work is to develop a phenomenological finite plasticity theory which describes the evolution of the anisotropy. We develop a framework of a general finite plasticity theory, some special cases are examined and the case of a so called Material Plasticity is examined more closely, assuming that the axes of anisotropy deform as material line elements. It will be applicable to, e.g.,

fiber reinforced materials. The main difference to a common plasticity theory is the different evolution of the stiffness tetrad and of the stress-free placement during a plastic deformation. For a verification of the results of this theory and to identify and compare the stiffness tetrads before and after large plastic deformations, a representative volume element (RVE) with a fibrous microstructure is used. Therefore we use the finite element program Abaqus and its scripting language Python. Uni-, bi- and and tri-directionally reinforced samples are considered. On the microscale, a finite elastic-plastic material model based on the concepts of isomorphy and maximum plastic dissipation is used. After calculating the effective stiffnesses of the different material samples, we investigate their evolution during different deformations. In addition, we present a fast algorithm to determine the distance of such a measured stiffness tetrad to all possible symmetries of an elastic stiffness tetrad. Therefore, we develop a projection method using an 8th-order tensor covering all group elements of the chosen symmetry group. Then it is necessary to find out how to predict the evolution of the stiffness tetrad. It turns out that it is possible to denote the change of the stiffness tetrad with sufficient accuracy using one additional 2nd-order tensor. We finally propose an analytical evolution equation for this tensor.

S06.2.02: Various topics in Material modelling with non-metals

Date: March 19, 2024 16:30–18:30
Room: G16/H5
Chair(s): Simon, Jaan-Willem
Lion, Alexander

Modelling material properties of composites using stochastic tensor approach

Schuttert, Wouter Jan; Abdul Rasheed, Mohammed Iqbal; Rosić, Bojana
University of Twente, The Netherlands
16:30

Materials like thermoplastic composites exhibit anisotropic behavior, and their characteristics may vary between the manufacturing samples due to inability to precisely control the manufacturing process. Due to lack of knowledge on this variation, one may incorporate the epistemic knowledge in the description of material properties by use of the probability theory. For this purpose one has to develop the stochastic model that may represent the material symmetry or its corresponding characteristics (e.g. constitutive parameters) as uncertain. To achieve this, one may model the material properties as symmetric and positive definite stochastic (SPD) tensors, the prior knowledge of which is described with the help of the maximum entropy principle. This talk focuses on the modeling of stochastic tensors of material properties such as thermal conductivity by use of the parametric approach [1]. The idea is to generate an ensemble of SPD tensors for which certain classes of spatial symmetries and invariances are prescribed together with the second order statistics of a possible higher spatial invariance class. We show that the parametrization of the model reduces to the so-called scaling and rotation related parameters that describe the uncertainties representing the corresponding symmetry class and orientation, respectively. The previously mentioned parameters are then modelled with the help of independent random variables on a manifold structure with the assigned probability distribution coming from the maximum entropy principle. To showcase the model, we apply the proposed approach on 2D and 3D numerical examples involving multiphysics problem such as induction welding of the thermoplastic composite.

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Notes on the Schapery model to describe non-linear viscoelastic phenomena

Margalho de Barros, Marcos Andre (1); Govindjee, Sanjay (2); Schröder, Jörg (1)
1: University of Duisburg-Essen
2: University of California, Berkeley, USA
16:50

Viscoelastic phenomena are present in every-day materials in engineering e.g., polymers, and bitumen materials. Materials like rubber present linear behaviour only if small deformations and small

perturbations from the thermodynamic equilibrium are imposed. Thus, collective effort has been set to develop a model that can describe these materials at large deformations, see [1]. Moreover, the viscoelastic non-linearity can be a consequence of the stress, temperature and/or ageing; therefore, the single-integral Schapery model [2], derived from thermodynamic theory of irreversible processes and implemented to investigate the non-linearity due to stress and temperature [3], is considered in this work.

The aim is to collect data from experimental models and fit them into the material functions and time scale shift factors. A finite element scheme for the Schapery model based on a stress-update algorithm is proposed. For this, the decoupled deviatoric and volumetric responses and the strain tensor decomposition into instantaneous and hereditary parts are carried out [4]. The Schapery model is expected to depict precisely the non-linear viscoelastic phenomenon in creep and recovery strain tests.

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Viscoelastic Constitutive Artificial Neural Networks (vCANNs) – a framework for data-driven anisotropic nonlinear finite viscoelasticity

Abdolazizi, Kian (1); Linka, Kevin (1); Cyron, Christian (1,2)

1: Hamburg University of Technology
2: Helmholtz-Zentrum Hereon

17:10

Finite linear viscoelastic (FLV) or quasi-linear viscoelastic (QLV) models are commonly used to model the constitutive behavior of polymeric materials. However, these models' limitations in accurately describing nonlinear viscoelastic phenomena, particularly in capturing strain-dependent viscous behavior, motivate the development of alternative methodologies. In response to this issue, we introduce viscoelastic Constitutive Artificial Neural Networks (vCANNs), a novel physics-informed machine learning framework. vCANNs rely on the concept of generalized Maxwell models with nonlinear strain (rate)-dependent properties represented by neural networks. With their flexibility, vCANNs can automatically identify accurate and sparse constitutive models for a wide range of materials. To assess the capabilities of vCANNs, extensive training was conducted using stress-strain data from synthetic and biological materials subjected to diverse loading conditions, e.g., relaxation tests, cyclic tension-compression tests, and blast loads. The results show that vCANNs can learn to accurately and efficiently represent the behavior of these materials without human guidance. We showcase the seamless integration of vCANNs into existing Finite Element codes through illustrative examples. This integration underscores the practical applicability of vCANNs in the field of applied mechanics.

A thermodynamically consistent physics-informed neural network model for nanoparticle-filled epoxy nanocomposites with moisture content

Bahtiri, Betim (1); Arash, Behrouz (2); Scheffler, Sven (1); Jux, Maximilian (3); Rolfes, Raimund (1)

1: Leibniz University Hannover
2: Oslo Metropolitan University
3: Institute of Lightweight Systems, Multifunctional Materials, DLR (German Aerospace Center)

17:30

Epoxy-based materials are frequently exposed to high-humidity environments in many engineering applications, resulting in material properties degradation. In this study, we develop a physics-informed neural network to predict the nonlinear viscoelastic/viscoplastic/damage behaviour for epoxy-based nanocomposites at finite deformation. In our previous work, we developed a long-short

term memory unit (LSTM)-based model [1] to replace the implicit time integration scheme and accelerate finite element (FE) simulations. The deep recurrent neural network (RNN) was adopted for the viscoelastic/viscoplastic modelling in the three-dimensional space and an accurate representation of the state variables. The predictive capability of the RNN model was evaluated using FE simulations. However, pure black-box data-driven models mapping strain to stress without considering the underlying physics suffer from unstable and unrealistic performance. Therefore, we propose a physics-informed neural network which predicts the stress-strain behaviour at finite deformations by considering the universal thermodynamics principles [2]. We train our model for the one-dimensional case to show that a physics-informed neural network can outperform a classical constitutive model. We perform experiments under cyclic loading-unloading conditions with moisture content at different temperatures and use these to calibrate the material model. The numerical results show an improvement of the accuracy compared to the classical approach.

Constitutive artificial neural network for elasto-plastic material behavior

Boes, Birte (1); Simon, Jaan-Willem (1); Holthusen, Hagen (2)
1: University of Wuppertal
2: RWTH Aachen University

17:50

The constantly advancing technologies in manufacturing processes allow to develop more and more new materials. To accurately predict their material behavior, novel material models and combinations of existing, sophisticated models need to be developed. So far, plenty of constitutive models exist that have been derived from the principles of thermodynamics. But for innovative material combinations, questions arise on which constitutive model should be chosen and how to formulate a novel accurate model. In order to facilitate finding of suitable new models, in this work, we make use of data-driven models using machine learning to predict the mechanical behavior by constitutive artificial neural networks (CANN). Promising results for elastic material behavior have already been described by Linka et al. [1], and an extension to visco-elastic behavior has recently been published by Holthusen et al. [2]. However, the extension to elasto-plastic material behavior is still open. Thus, we propose a novel formulation of constitutive artificial neural network, based on the mentioned works above, that can be applied to elasto-plasticity by combining feed-forward networks of the Helmholtz free energy and the yield function. Physical information such as stress-strain data and conditions from materials theory will be incorporated, such that the resulting physics-informed CANN directly results in constitutive models that fulfill the principles of thermodynamics *a priori*. As a result, this work introduces a novel formulation of constitutive artificial neural network that captures elasto-plastic material behavior.

References

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[2] H Holthusen, L Lamm, T Brepols, S Reese, E Kuhl: Theory and implementation of inelastic Constitutive Artificial Neural Networks. *arXiv preprint arXiv:2311.06380*, 2023.

S06.2.03: Various topics in Material modelling with non-metals

Date: March 20, 2024 16:30–18:30
Room: G16/H5
Chair(s): Holthusen, Hagen
Kehrer, Loredana

Design and application of inelastic Constitutive Artificial Neural Networks (iCANN)

Holthusen, Hagen (1); Lamm, Lukas (1); Brepols, Tim (1); Reese, Stefanie (1); Kuhl, Ellen (2)
1: RWTH Aachen University
2: Stanford University, USA

16:30

Centuries of physics have led us to uncertainty-free conversational laws of solids in a continuum mechanical context. These principles of thermodynamics are valid regardless of the specific material

behavior of interest. Deduced from these principles, several material models for hyperelastic materials have been derived that satisfy these principles. However, in contrast to these principles, the ability of certain models to describe different materials is limited. Usually, we pre-select a material model to fit the experimentally obtained data. This implies the intrinsic problem that we may have already chosen a model that is inadequate. This is already problematic for elasticity and is even worse for inelastic material behavior. To circumvent this, machine learning algorithms are best suited to learn the best possible model to explain the data. However, these can suffer from unphysical behavior, especially for prediction. Therefore, several years ago, a family of Constitutive Artificial Neural Networks [1-2] was developed that combines thermodynamic knowledge with modern machine learning techniques. These networks are designed to satisfy thermodynamics a priori, but are limited to elastic behavior. The question is how to extend them to inelastic materials. One general way to do this is to introduce a pseudo potential in the form of the thermodynamic driving force associated with the inelastic rate [3]. Here we extend CANNs to inelastic material behavior (iCANN) [4-5]. Therefore, our network learns both the Helmholtz free energy and the pseudo potential. Thus, thermodynamics is still satisfied a priori regardless of the inelastic phenomena. With the help of iCANNs, the various inelastic phenomena hidden in the experimental data, such as plasticity, viscosity, degradation, growth and remodeling, may be identified and revealed to us. Here, we demonstrate that our iCANN is capable of discovering a model for the visco-elastic behavior of polymers and skeletal muscle data.

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Exploring the possibilities of physically enhanced neural networks in advanced material modeling

Maurer, Lukas; Eisenträger, Sascha; Juhre, Daniel 17:10
Otto von Guericke University Magdeburg

Neural networks (NN) often refer to constructs that can process large amounts of data and attempt to find relationships between different variables. A prominent example is user data from social networks (interactions) being used to determine user preferences. Based on the collected data, automatically adapted user-specific advertising is created. In addition to such almost purely data-driven approaches, NNs have increasingly become the focus of physically motivated research problems in recent years.

Classical feed-forward NNs provide accurate interpolation functions, but most of them are very poor at extrapolation. Another problem is related to the networks sensitivity towards noisy experimental data, which results in a poor performance due to a misplaced focus on deviations in the training set during training. In addition, in most cases the network has to learn the known physical principles from scratch. However, it has been shown that the neural network can be forced by its construction to fulfill some bounds for the specific output variables. Here, the choice of input and output variables can also have a major influence. Derived variables, such as invariants, can be used as input variables and automatic differentiation (AD) can be utilized to calculate the change in all related quantities. PINNs (physically informed NNs) are a second approach that heavily relies on AD. Differential relations can be trained here in a softer way, as additional points outside the training set are employed to create a second loss function defined by a differential equation rather than by the error between calculated or measured targets and the network output.

This contribution looks at these physically motivated neural network approaches in the field of material modeling. Besides a discussion on the selection of the best input and output variables, physical

axioms such as the non-negativity of the strain energy function or the use of invariants as input variables of the network are also considered in the construction and training of the NNs. In addition to insights regarding the derivation of elastic and hyperelastic materials based on a small amount of data, the creation of a viscoelastic material model is presented. The trained networks are then used in a three-dimensional finite element framework and compared with classical material models in terms of accuracy and computational effort.

How to incorporate physical information into ANNs by physics-based Rao-Blackwellization: Example of isotropic rubber elasticity

Geuken, Gian-Luca; Kurzeja, Patrick; Mosler, Jörn 17:30
TU Dortmund University

Artificial neural networks (ANNs) and data-driven approaches recently have gained widespread popularity for solving computational problems. This is also the case for the modeling and simulation of polymers exhibiting complex non-linear material behavior. Modeling such behavior can be challenging, in particular for complex or noisy experimental data. In this context, ANN models emerge as fast, efficient and highly flexible alternativesto classical models.

Recent advances underline the enhanced performance of ANNs through the integration of physical insights. 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. It can be proven that the improved estimator yields a smaller or equal mean-squared-error compared to the initial estimator, making Rao-Blackwellization a powerful method even for coarse data sets. To be more precise, it utilizes sufficient physical information for a material model, replacing the statistical modeling framework of the original algorithm. This new method moreover complements other approaches such as physics-informed neural networks (PINNs) [2] and constitutional artificial neural networks (CANNs) [3], still preserving the optimality condition.

Different facets and benefits of the proposed method are discussed, using isotropic rubber elasticity as a case study. Beginning with raw DIC data from a tensile experiment of 3D-printed Thermoplastic Polyurethane (TPU), we impose multiple constraints, such as isotropy, material invariance and differentiability, to guide the augmentation of ANN training data. In addition, we present how an implementation of physically sound constraints into an ANN leads to poorer predictions, if the constraints impair the underlying scheme. The talk concludes with a comparison of finite element simulations using the ANN models against experimental reference, highlighting the importance of a sophisticated improvement scheme.

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neural networks: a guaranteed improvement via physics-based Rao-Blackwellization. 2023. https://doi.org/10.48550/arXiv.2311.06147

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An expanded model for the evolution of olivine crystals

Haddenhorst, Hendrik Holger; Chakraborty, Sumit; Hackl, Klaus 17:50
Ruhr University Bochum

In this presentation, we discuss the material model introduced by Haddenhorst et al. [1] 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. [1]

Thanks to this model, it is possible to make predictions about the stability of such crystals based on the environmental conditions. The results of our investigation with regards to the stability are presented, and we discuss possible ways to expand model to improve its accuracy and widening its scope of applications.

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[1]: Haddenhorst, H. H., Chakraborty, S., & Hackl, K. (2023). A model for the evolution size and composition of olivine crystals. Proceedings in Applied Mathematics and Mechanics, 00, e202300081. https://doi.org/10.1002/pamm.202300081

Identifying Fiber Orientation and Fiber Volume Fraction Distributions in a Commercial Paperboard for Computational Modelling

Kloppenburg, Greta (1); Li, Xiangfeng (1); Dinkelmann, Albrecht (2); Finckh, Herrmann (2); Neumann, Johannes (1); Simon, Jaan-Willem (1)

1: University of Wuppertal
2: German Institutes of Textile and Fiber Research Denkendorf

18:10

Paper and paperboard are commonly utilized as writing, printing, and packaging materials. Nonetheless, paper's exceptional mechanical properties and excellent recyclability make it a viable substitute for classic engineering materials such as metals or plastics.

This is due to the microstructural fiber network present in paper which strongly impacts macrostructural properties, including in- and out-of-plane anisotropy, as well as tear strength. Macrostructural issues such as problems with folding processes or package instability are often associated with this network, specifically the fiber volume fraction and orientation. While there is extensive research on paper composition, the distribution of fiber orientation and volume fraction remains poorly understood. Although these distributions are intriguing per se, they hold significant value as input data for computational models on a network scale.

Therefore, gaining a more profound understanding of the microstructure through non-destructive imaging methods is worthwhile. These methods have proven effective in numerous applications with various materials in the past. We examined a three-layered paperboard, with a grammage of 240 g/m^2, intended for packaging liquids, to investigate its fiber distribution. Forty samples from both edge and center positions of a single paper roll have been extracted, to observe the microstructural disparities within the roll. Thereafter, we conducted micro-CT scans, which yielded data on the entire paper thickness. After segmenting and identifying individual fibers, their orientations were described through orientation tensors for cell sizes of 500x500x2 microns.

The analysis computed the principal directions for over 20,000 cells/orientation tensors, revealing that the fibers are predominantly aligned in-plane. There are no notable differences in out-of-plane anisotropy between center and edge positions. However, center positions in the paper roll exhibit a larger in-plane scatter. The fiber volume fraction tends to be higher in the top and bottom layers of the paperboard compared to the middle layer.

Parameters for multiple non-periodic and periodic probability density functions were established via the use of a maximum likelihood method. The goodness of fit for parametrized probability density functions was evaluated, and the top-performing candidates were identified. These functions will be implemented in the future for generating network models for computational analysis.

S06.2.04: Various topics in Material modelling with non-metals

Date: March 21, 2024 08:30–10:30
Room: G16/H5
Chair(s): Bohnen, Matthias
Kehrer, Loredana

Mechanical data acquisition for microgels

Khiêm, Vu Ngoc; Choudha, Ambuj; Itskov, Mikhail 08:30
RWTH Aachen University

Microgels are cross-linked polymer networks at the micrometer scale, exhibiting a state of swelling in a solvent. They possess a number of promising properties, such as biocompatibility, environmental friendliness, adhesion, antibiofouling behavior, and biodegradability. However, the small dimensions of microgels pose challenges in the acquisition and analysis of mechanical data, thereby necessitating specialized methodologies for comprehensive investigation. In this contribution, computer vision is coupled with *in situ* microscopy on a single microgel to collect real mechanical datasets at the micrometer scale. A deep convolutional neural network will be designed to detect deformation field from image inputs. The efficacy of its predictions will be illustrated through the utilization of both *in silico* and real experimental data.

Remarks on parameter identification using finite elements and full-field data

Hartmann, Stefan (1); Römer, Ulrich (2); Wessels, Henning (2); Tröger, Jendrik-Alexander (1) 08:50
1: Clausthal University of Technology
2: TU Braunschweig

The parameter identification problem on the basis of finite elements using least-squares in combination with full-field data, for example, digital image correlation data to provide the deformation fields, is more or less well established. It can be treated either by the so-called reduced formulation or by the all-at-once approach. The basic differences become apparent if the constitutive models are formulated as elastic or inelastic on the basis of evolution equations.

In the presentation, the forward or direct problems using finite elements are discussed first within the method of vertical lines, i.e. the clear treatment of space and time discretization. Afterwards, the frequently so-called reduced formulation is discussed, where the finite element results are directly compared to the experimental data. In this context, it becomes clear that the implicit function theorem is exploited. Then, the entire scheme is compared to the so-called all-at-once approach where both the equilibrium conditions, or the resulting system of differential-algebraic equations, are minimized on the same level as the residual between the state, i.e. the unknown displacements and reaction forces, with the experimental data of the full-field data or the force gauge information of the testing machine.

It is tried to clearly distinguish the unknowns, prescribed nodal displacements, and reaction forces. The advantages and disadvantages of the methods are worked out. Furthermore, it is compared to the virtual field method.

Process simulation for thermal powder bed fusion additively manufactured glasses based on the Hamilton principle using Neigbor Element Methode (NEM)

Rudolf, Tobias; Soleimani, Meisam; Bode, Tobias; Junker, Philipp 09:30
Leibniz University Hannover

Glass has various physical properties that make it a versatile material in industry. These properties are particularly important in the field of optics. Material properties such as thermal and chemical resistance, electrical insulation and hardness should be emphasised and distinguish glass from transparent plastics. In the production of high-performance lenses in the field of optical lasers, the requirements for precision and flexibility in shaping are constantly increasing. To meet these requirements, additive manufacturing processes are becoming increasingly important. Despite the large number of manufacturing processes, high temperatures are usuallyrequired to bring the starting material into the desired shape. The temperature and its gradients significantly influence the material properties of glass during the phase transformation. The local fusion of material at the interface between the particles taking place at high temperatures is a multiphysics process in nature. The mathematical model of multi-field problems is challenging due to thermodynamics-dictated principles. In order to fulfill the thermodynamic consistency, an extension of the Hamilton principle is employed to drive the

governing differential equations. The evolution equations and corresponding driving forces formulated within this framework are thermo-mechanically coupled. A hybrid strategy based on both finite elements and mesh free finite differences methods is utilized to numerically implement the mathematical model. This procedure is called the Neigbhored Element Method (NEM). The numerical code is implemented in the ANSYS software environment. The aim is to simulate the phase transformation of glass during additive manufacturing processes. The influence of different temperature gradients and different process parameters should be taken into account. Such numerical tool provides insights into controlling the design parameters of 3D printed parts such as unwanted distortions, residual stresses and desired mechanical stiffness.

One-point integration for T2 elements in viscoelasticity

Choi, Yongbin; Bode, Tobias; Junker, Philipp
Leibniz University Hannover

09:50

Simulating the behavior of materials with microstructure evolution is complex and the simulation time can be significantly longer compared to elastic materials. The reason for this is that the state of the microstructure changes with time and load and therefore evolution equations have to be solved at each quadrature point at each time the residual or tangent matrix is computed. Reducing the simulation time while maintaining the accuracy of the results is a very important and interesting topic nowadays. In this work, the 1-point quadrature method for the behavior of viscoelastic material for 6-node triangular elements (T2 elements) is investigated. Hyperelastic materials have already been simulated in previous studies (Bode 2023 [1]) using the 1-point quadrature method for higher order elements and have shown good results.

The evolution equation for viscoelasticity can be derived, for example, using Hamilton's principle (Junker et al. 2018 [2]). Using the non-conservative model, the virtual strain energy can be approximated by a Taylor series expansion of the stress with respect to the strains. In turn, the strains can be expanded with respect to the spatial terms. The geometric moments required for the one-point integration can be calculated via a surface integral in preprocessing. By using 1-point integration, the viscoelastic evolution equations only have to be evaluated at a single point per element, despite the higher order approach. The investigation of time efficiency in terms of assembly time while maintaining accuracy in the integration is investigated.

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Topology optimization for precipitation hardening in ferroelectric material

Bohnen, Matthias; Müller, Ralf
TU Darmstadt

10:10

Precipitation hardening is a well known heat treatment to enhance the mechanical properties of metals. However, this technique can also be applied to ferroelectric crystals, as recent studies have shown. As an alternative to doping, it effectively reduces domain wall mobility as well as heat dissipation and by that enhancing the mechanical quality factor of ferroelectric materials. Determining the optimal shape and size of the precipitates represents a question of active research with the goal to improve the efficiency of ferroelectric material. This work aims at optimizing the geometry of precipitates inside their matrix by minimizing the total energy resulting from bulk and interface contributions. We compare different geometrical approaches with elliptical shapes and interfaces defined by splines. The model is later on extended by an established phase field approach to simulate the

polarization field in ferroelectric material. The pinning effect of precipitates on domain walls is analyzed with finite element computations. This allows to determine favorable shapes and distributions of precipitates.

S06.2.05: Various topics in Material modelling with non-metals

Date: March 21, 2024 17:40–18:40
Room: G22/013
Chair(s): Christ, Nicolas
Lion, Alexander

Mesoscopic Structure Modeling of Flexible Macroporous Aerogels using Cluster-Cluster Aggregation

Xiong, Weibo; Abdusalamov, Rasul; Itskov, Mikhail 17:40
RWTH Aachen University

Organosilane-derived aerogels have generated considerable interest for their capability to confer specific chemical functionalities, such as hydrophobicity and flexibility. This study examines the structure modeling of flexible, opaque aerogels made from organoalkoxysilanes.

The pH of sol-gel polymerizations is one of the most critical reaction and processing parameters in determining the porosity, density, strength, and transparency of resulting gels. Achieving optical transparency in aerogels depends on the presence of homogeneous, mesoporous network structures. To account for the effect of pH, a connection between pH and sticking probability was incorporated into a three-dimensional cluster-cluster aggregation (CCA) model, providing insight into the gelation process. Additionally, this study considers size-dependent diffusivities. Furthermore, an exploration into modeling phase separation in gels is undertaken, assuming the existence of impurities.

By incorporating different factors into the CCA model, we assess their impact on gelation kinetics. The obtained mesoscopic structure is compared to experimental characterizations, together with preliminary mechanical simulations, marking the first step for upcoming research.

Double-surface plasticity for a micropolar continuum

Börger, Alexander; Mahnken, Rolf 18:00
Paderborn University

This work is concerned with the modeling of a cold-box sand, a composition of sand grains and a resin binder. To this end, experiments are performed which show the following characteristics: localization phenomena in form of a shear band, softening behaviour in the force-displacement curve, asymmetric behaviour for compression and tension. These complex characteristics require a sophisticated material model. For this purpose a micropolar continuum, which is a special case of the micromorphic continuum, is used. In addition to the degrees of freedom of a classical continuum, the micropolar model has additional degrees of freedom in the form of micro-rotations, which represent the grains of sand in our analysed material. The macro-part of this model represents the binder of the cold-box sand. In order to make the micropolar model as flexible as possible, two flow functions are introduced; one for the macro-part and one for the micro-part. These two flow functions can be implemented independently or coupled, depending on the application. For the coupled case, the radial-return algorithm is no longer sufficient, so that the local iteration is calculated with the Fischer-Burmeister residual. Due to the lack of rotational symmetry in the experimental results, it is not possible to compute in two dimensions; instead, a 3D model is used for the simulation.

Computational Modelling of Non-Woven Material Compression

Wan, Chengrui (1); Heider, Yousef (1,2); Markert, Bernd (1) 18:20
1: RWTH Aachen University
2: Leibniz University Hannover

This research presents a computational model designed to simulate the compression of non-woven materials composed of entangled, non-cross-linked fibre systems. These materials undergo varying

compression states, notably during processes like needle-punching in their production [1]. Understanding the microstructure at different compression states is crucial for accurately simulating the macroscopic behaviour of non-woven materials in such scenarios.

To address this, a discrete computational model treating fibres as chains of interacting spheres is proposed. A quasistatic, uniaxial load is incrementally applied to achieve the target compression state. The numerical implementation, utilising force-based dynamics for discrete particles, incorporates recovery forces originating from the fibre elasticity and repulsive forces at the contact sites of the fibres. The frictional behaviour of the fibres is also described in the numerical model. The algorithm has been optimised for enhanced computational efficiency when simulating a large number of fibres.

The model allows for the virtual compression of the fibre system, enabling the simulation of final configurations at any compression state, given the initial fibre topology and relevant material parameters. Furthermore, it provides a load-compression relationship, thereby serving as a homogenization method for understanding the mechanical behaviour of such microstructural materials.

References:

[1] Archut, J.-L.; Kins, R.; Heider, Y.; Cloppenburg, F.; Markert, B.; Gries, T.; Corves, B. A Study of the Mechanical Response of Nonwovens Excited by Plate Vibration. Appl. Mech. 2022, 3, 496-516. https://doi.org/10.3390/applmech3020029

S06.2.06: Various topics in Material modelling with non-metals

Date: March 22, 2024 08:30–10:30
Room: G16/H5
Chair(s): Juhre, Daniel
Lion, Alexander

How to Identify the hardening curve of PVDF films from tensile tests and simple shear tests for application in adhesive bondline modelling

Kilian, Riem; Völkerink, Oliver; Steinmetz, Julian; Hühne, Christian 08:30
TU Braunschweig

For elastic-plastic material modeling, it is essential to determine a hardening curve. This study compares the hardening curves from tensile test and simple shear tests for modelling a epoxy bondline with surface toughening elements. Surface toughening implies the local integration of poly(vinylidene fluoride) (PVDF) film at the overlap ends on the adherend surface. From the conventional method using tensile tests follows the assumption that the material model is more accurate when determining a hardening curve from tests with the same dominate load case as the application. Thus, simple shear tests might be more suitable to identify the hardening curve of adhesive bondlines, where shear stresses dominate. The motivation for precise hardening curves originates from the multimaterial bondline. In this study, a thermoplastic PVDF film is investigated, which can be used as surface toughening in structural adhesive joints to decrease peel stresses at the overlap-ends. To verify the influence of the load case on the hardening curve, tensile tests as well as simple shear tests are carried out. In contrast to tensile tests, integrating the hardening curve into finite-element software, such as ABAQUS, presents challenges in the context of simple shear loading. For the integration, the plastic strain and engineering stress need to be formulated as von Mises equivalent strain and stress in terms of true strain and stress components. However, for simple shear, converting the engineering stress tensor (first Piola Kirchhoff stress) into the true stress tensor (Cauchy stress) is challenging. This difficulty mainly comes from potential additional principal stress components that are unknown due to inhomogeneous deformation. This work proposes an approach to determine the hardening curve from a simple shear test that can be imported into ABAQUS using thick adherend shear tests. The experimental results are stress-strain curves. Then the yield stress is determined by employing different criteria. One common method is the definition of yield when the proportional limit with an 0.2 % offset of plastic strain is reached. An alternative proposes to define the yield point as the point at which the rate of the tangent modulus in the stress-strain curve is maximized. Subsequently, the

conversion from the first Piola Kirchhoff stress to Cauchy stress is addressed based on the assumption of small deformation. By comparing the nominal strain with the true (Henky) strain t is possible to prove quantitatively small deformations. This enables the simplification of the simple shear stress tensor, so that a conversion to true stress and strain measures is not absolutely necessary. The comparative analysis of the hardening curves obtained from tensile and simple shear tests indicates that the PVDF film is more ductile under simple shear load. Moreover, the hardening differ significantly depending on the yield criteria.

Thermoviscoelastic modeling and simulation of enthalpy relaxation in thermoplastic polymers

Keursten, Johannes; Enders, Sabine; Böhlke, Thomas 08:50
Karlsruhe Institute of Technology

Thermoplastic polymers are used in a wide range of industrial applications. Due to their potential as cost-efficient lightweight materials, thermoplastics, e.g., serve as matrix material in fiber reinforced composites [1]. Thermoplastics exhibit a glass transition from a glassy to an equilibrium state within the temperature range of application. Thus, the glass transition is a crucial point in thermomechanical modeling of thermoplastics.
The focus of this work is on the process-dependent caloric behavior in the vicinity of the glass transition. In differential scanning calorimetry (DSC), the heat capacity decreases monotonically in cooling processes and it increases non-monotonically in heating processes. The latter phenomenon is known as enthalpy relaxation [2,3]. Enthalpy relaxation is captured by the thermoviscoelastic Poynting-Thomson model including thermal expansion and an additional caloric relaxation equation [3]. In this framework, temperature dependency of the relaxation times is modeled by time-temperature superposition, e.g., the WLF equation. This work will demonstrate how the model can be fitted to experimental measurements of the heat capacity. As an example, DSC measurements of polystyrene at various temperature rates are considered. Based on further numerical simulations, the qualitative and quantitative behavior of the thermoviscoelastic and caloric parts of the model are discussed regarding various temperature loadings.

References

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Effects of Temperature and Humidity on the Interfacial Shear Strength of Carbon Fiber Reinforced Polyamide 6: Insights from Single Fiber Pull-Out Tests and Finite Element Analysis

Christ, Nicolas (1,2); Montesano, John (3); Hohe, Jörg (2) 09:10
1: Karlsruhe Institute of Technology
2: Fraunhofer IWM
3: University of Waterloo, Canada

Fiber-reinforced thermoplastics offer high specific stiffness and strength combined with good recyclability and are becoming increasingly important for resource conservation and environmental sustainability. Among these, carbon fiber reinforced polyamide 6 has emerged as a material of considerable interest. Understanding the fiber-matrix adhesion behavior in these materials is crucial for their effective utilization. At the same time, since thermoplastics are susceptible to creep effects even at low temperatures, and considering the hygroscopic nature of Polyamide 6, the effects of environmental conditions such as temperature and humidity need to be thoroughly investigated. This study aims to evaluate these effects on material performance. A dual approach combining single fiber pull-out tests under different environmental conditions and numerical investigations using Finite Element Analysis (FEA) is employed. The nonlinear parameters of the matrix, which are essential for understanding its

viscous behavior, are determined by micromechanical creep tests. These parameters are then integrated into Schapery's nonlinear viscoelastic model (Schapery, R., 1969) for a more comprehensive analysis. Although results are pending, the research anticipates a significant influence of environmental factors on both the interfacial shear strength and the viscous behavior of the matrix. It is expected that this work will provide valuable insight into the role of the fiber-matrix interface under various environmental conditions, thereby contributing to a broader understanding of fiber-reinforced thermoplastics.

Hydrothermal behavior of PA 6 reinforced with discontinuous long carbon fibers

Kehrer, Loredana (1); Scheuring, Benedikt (2); Blarr, Juliane (2); Böhlke, Thomas (1)
1: Karlsruhe Institute of Technology, Institute of Engineering Mechanics, Continuum Mechanics
2: Karlsruhe Institute of Technology, Institute for Applied Materials

09:30

Polymer-based composites play a crucial role in the lightweight sector as they represent resource-efficient semi-structural materials. Herein, polyamides serve as widely-used matrix materials for fiber-reinforced composites in diverse technical applications [1]. The mechanical behavior and technical performance of polyamide 6 (PA 6) are profoundly influenced when exposed to environmental conditions such as temperature and humidity [2,3]. Previous studies have examined the effect of hydrothermal conditions on the mechanical properties of pure PA 6, as documented in [4]. The aim of this work is to extend the scope of the previous investigations by the inclusion of discontinuous (DiCo) long carbon fiber-reinforced PA 6. Experimental tests are performed to examine the impact of fibers on the hydrothermal mechanical behavior, revealing the complex interplay between environmental factors and composite material performance. To enhance the understanding, a micromechanical approach is employed to consider the microstructure of the DiCo carbon fiber-reinforced PA 6. The study incorporates a mean-field approach for homogenization, enabling a systematic analysis of the composite's mechanical response. A validation based on experimental investigations ensures the practical applicability and robustness of the developed model and contributes to valuable insights for optimizing the performance of PA 6 in fiber-reinforced composites under varying environmental conditions.

References

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S07: Coupled problems

Organizer(s): Schröder, Jörg *(University of Duisburg-Essen)*
Düster, Alexander *(Hamburg University of Technology)*

S07.01: Phase-field models

Date: March 19, 2024 08:30–10:30
Room: G16/215
Chair(s): Reichel, Maximilian
Krischok, Andreas

A Framework Incorporating Rate-Independence in Phase-Field Modeling with Application to Hysteretic Effects in Shape Memory Alloys

El Khatib, Omar; von Oertzen, Vincent; Kiefer, Bjoern 08:30
TU Bergakademie Freiberg

Shape memory alloys (SMAs) represent a unique class of multifunctional materials, known for their remarkable thermo-mechanical properties. These materials exhibit the exceptional ability to recover their original shape under specific stress and temperature conditions. This characteristic stems from microscopic phase transformation mechanisms, involving a reversible transition between austenite and multi-variant martensite. Moreover, the formation of remanent microstructures in SMAs during cyclic loading gives rise to a hysteretic behavior, representing the energy dissipated during each transformation cycle. As observed in experiments for a wide range of SMAs, resulting stress-strain and undercooling curves suggest a rate-independent response to quasi-static loading, so that hysteresis loops obtain a finite width even as the external loading rate approaches zero. Over the past few decades, the phase-field method has emerged as a powerful modeling framework, effectively capturing and resolving the evolution of complex interface topologies in phase-transforming solids. This capability has enabled a deeper understanding and accurate prediction of the hysteretic behavior of SMAs, a key aspect for their efficient utilization in various engineering applications. Despite many important scientific contributions in this regard, see [1] and the references therein, most existing models employ rate-dependent dissipation formulations, thus limiting their ability to accurately replicate thermo-elastic hysteresis loops under quasi-static loading conditions.
To address these limitations, this work extends a recently introduced thermomechanically coupled and variationally consistent Allen-Cahn phase-field approach that incorporates both rate-dependent and -independent driving force formulations, see [2]. Furthermore, by incorporating continuously distributed and temperature-dependent local energetic minima within the underlying free energy landscape, the proposed framework effectively captures sigmoidal-like undercooling hystereses as well as stress- and temperature-induced martensite pattern formation. To demonstrate the practical applicability of the outlined approach, two-dimensional finite element simulations are conducted to study the microstructure formation of twinned martensite in SMA systems. In this regard, the evolution of remanent microstructure under cyclic undercooling conditions—which is crucial for understanding the long-term behavior of SMAs—is investigated subject to repeated thermal and mechanical loading cycles. These studies include the analysis of rate-dependent and -independent stress- and temperature-induced hysteresis loops, the influence of model-specific driving force threshold values as well as the calibration of additional system parameters with experimentally observed martensite start and finish temperatures.

References:

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Modeling of interface elasticity within Allen-Cahn type phase field theory

Wilbuer, Hendrik; Kurzeja, Patrick; Mosler, Jörn 08:50
TU Dortmund University

Phase field modeling has been established in continuum mechanics as an important tool for simulations in various fields like fracture or microstructure modeling. In the present work, a framework for the latter has been implemented, which is capable of handling mechanically-induced phase transformations in time and space. In contrast to previous works, the focus is placed on deformation-dependent hyperelastic material interfaces – in line with surface elasticity theory as originally introduced by Gurtin and Murdoch.

By embedding the model into a finite element framework, effects of the deformation-dependent material interfaces on displacive phase transformation (Allen-Cahn type) will be presented and discussed using numerical examples.

A coupled approach for generalized hyperelastic continua and phase fields

Doghman, Jad; Ask, Anna; Bovet, Christophe 09:10
ONERA, France

When it comes to modeling and illustrating complex internal structures such as granular or fibrous materials, the Cosserat theory comes into view. To take into account the grain boundary motion in recrystallization processes, the Cosserat theory is adapted with inspiration from orientation phase-field models. The implementation of such a combination is challenging on account of its complexity for three-dimensional frameworks involving large deformations. In this work, a computational framework that takes into account a hyperelastic material law based on finite strain and curvature in three dimensions, coupled with a phase-field model, has been considered and numerically discretized through a fully non-linear finite element formulation and an implicit Euler method. A Newton-Raphson algorithm is then employed in order to compute the nodal displacements and rotations, which together form a six-degree-of-freedom system. For the resolution of the temporal and spatial evolution of the phase-field model, which represents one additional degree of freedom, an alternating minimization scheme, borrowed from the convex optimization field, has been made use of. By adopting such a scheme rather than solving a monolithic system, some ill-conditioning of the system stiffness matrix can be avoided. Compared to a classical continuum description, the presence of additional degrees of freedom (seven as opposed to three) implies longer simulation times. Still, compared to other simulation approaches that have been proposed for recrystallization, the entire microstructure can here be represented via only the three additional degrees of freedom. It is worth noting that, unlike the displacement part which does not suffer from defectiveness, rotation compounds have undergone a parametrization process; namely a Wiener-Milenkovic parametrization, in order to avoid singularities and to enable more than one complete turn per node. Observe that two different rotation types can coexist within the studied problem: a micro-rotation stemming from the Cosserat theory and a macro-rotation emerging from the classical continuum mechanics. To associate the microrotation with the crystal orientation, both rotations are assumed to coincide through the imposition of a penalty parameter. The proposed numerical scheme is implemented in the Z-set software which is based on the C++ language. The convergence of the proposed numerical scheme is accomplished without any instabilities. The correctness of the considered model, its discretization as well as its implementation are justified through comparisons with small deformation-based models.

FE-Implementation and Application of a Fully Coupled Chemo-Mechanical Phase-Field Model

Roth, Stephan; Seupel, Andreas; Kiefer, Bjoern 09:30
TU Bergakademie Freiberg

The inevitable energy transition and the transformation towards the use of hydrogen is currently motivating and accelerating research and development in the field of chemo-mechanically coupled material modeling and simulation technologies, as chemical reactions and diffusion must increasingly be taken into account in the design of components, especially in the energy and automotive sectors.

Reliable, robust and efficient simulation tools are a necessary prerequisite for this process. Against this background, we want to present the implementation of a fully-coupled chemo-mechanical phase-field model for reactive multi-component and multi-phase systems as a user-defined finite element (UEL) for the FE software Abaqus. The multi-field model that was implemented is founded on the general framework of Svendsen et al. [1], which was recast into a mixed variational formulation according to Miehe [2, 3]. It accounts for the coupling of mechanical deformation to additional microprocesses that influence the chemical composition, phase-state, and diffusion. More specifically, we incorporate chemical reactions [3], concentration-dependent swelling deformations [4], inelastic strains related to phase transformations as well as phase-dependent elastic properties. The presented numerical implementation utilizes UELlib, a library of Fortran modules for FE formulations, which allows for a general and flexible definition of user elements. In order to demonstrate the capabilities of the numerical framework, a set of 2D and 3D model problems, such as generalized Cahn-Hilliard and Allen-Cahn problems, is presented and discussed w.r.t. modeling effort and numerical efficiency.

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On the behaviour of a phase field model for wetting on sinusoidally shaped surfaces

Kunz, Jana (1); Hasse, Hans (1); Müller, Ralf (2)

1: RPTU Kaiserslautern-Landau
2: TU Darmstadt

09:50

Technical surfaces are generally not perfectly smooth, but usually exhibit roughness. Additionally, as micro-production techniques continue to evolve, geometrical surface structures at the micro scale can be manufactured, which presents a challenge for wetting models that are commonly formulated for smooth surfaces.

In [1, 2], a phase field model for surface wetting was proposed that serves as a basis for this investigation. On smooth surfaces, the width of the gas-liquid interface can be widened for scale bridging purposes, as this allows for accurate computations on coarse grids [3]. However, it was observed that this interface scaling impacts the results when the model is applied to rough surfaces [4], and therefore a free choice of the interface width is not always sensible.

In this work, the ability of the model to deal with sinusoidally shaped surfaces is investigated. An Allen-Cahn evolution equation is used to determine static equilibrium configurations for droplets on such surfaces.

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Phase separation in metal hydrogen systems predicted by Cahn-Hilliard type phase-field simulations

Dyck, Alexander (1); Wagner, Stefan (2); Pundt, Astrid (2); Böhlke, Thomas (1) 10:10
1: Karlsruhe Institute of Technology, Institute of Engineering Mechanics - Chair for Continuum Mechanics
2: Karlsruhe Institute of Technology, Institute for Applied Materials - Materials Science and Engineering

Storing hydrogen in stabilized small-sized metal-hydrogen systems (such as Palladium-Hydrogen) is a promising way to achieve fast loading and extraction rates due to the small length scales. In bulk systems, Palladium typically forms a hydride upon hydrogen absorption, leading to a two-phase system of hydrogen-poor alpha-phase and hydrogen-rich hydride. However, in stabilized small-sized systems, due to the boundary conditions mechanical stresses and elasto-plastic deformations drastically change hydrogen absoprtion and hydride formation [1].

In order to understand the coupling of hydride formation and elasto-plastic deformations in small-sized metal-hydrogen systems, chemo-mechanical models can be helpful. In this talk, we use a Cahn-Hilliard type phase-field theory for hydrogen diffusion coupled to elasto-plastic deformations in order to study hydrogen uptake and hydride formation, using the Palladium-Hydrogen system as an example. We present the thermodynamically consistent constitutive theory as well as an implementation in a finite element seeting [2] using the Finite-Element software ABAQUS. We show, that depending on the mechanical behavior of the metal, elasto-plastic deformations indeed change the metal's capacity to form hydrides.

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S07.02: Laser beam welding

Date: March 19, 2024 16:30–18:30
Room: G16/215
Chair(s): Scheunemann, Lisa
Gumenyuk, Andrey

Determination of critical local straining conditions for solidification cracking at laser beam welding by experimental and numerical methods

Bakir, Nasm (1); Gumenyuk, Andrey (1); Rethmeier, Michael (1,2,3) 16:30
1: Bundesanstalt für Materialforschung und-prüfung (BAM), Berlin
2: Fraunhofer IPK
3: TU Berlin

The phenomenon of solidification cracking has been the subject of numerous research projects over the years. Great efforts have been made to understand the fundamentals of hot cracking. It is generally agreed that solidification cracks form in the solidification range between the liquidus and solidus temperatures under the combination of thermal, metallurgical and mechanical factors. There is still a need to determine the time-resolved strain distribution in the crack-sensitive region in order to analyze the local critical conditions for solidification cracking phenomena. This was a strong motivation for the development of a measurement system used in this study to estimate the local strains and strain rates in the zone where the solidification crack is expected to occur. The laser beam welding experiments were conducted using the Controlled Tensile Weldability test (CTW test) to apply an external strain condition during welding to generate solidification cracks. The CTW test is a test method for investigating the susceptibility of laser-welded joints to solidification cracking, in which the sample can be subjected to a defined strain at a defined strain rate during welding.

In combination with experimental investigations, numerical simulations provide spatially detailed and time-dependent information about the strain development during the welding process, especially regarding the critical conditions for solidification cracking. Therefore, this tool was also used in the present study to evaluate the accuracy of measurement methods and to estimate experimentally derived values and their concrete influence on the formation of solidification cracks. By integrating experimental methods and numerical simulations, this study investigates the spatially resolved and temporally changing development of strain during welding, with a particular focus on the critical conditions that lead to the formation of solidification cracks. The use of numerical simulations serves a dual purpose by validating the accuracy of measurement methods and examining experimentally determined values for their actual influence on the formation of solidification cracks. A three-dimensional finite element (FE) model implemented with ANSYS is used to simulate strains and stresses during welding. The credibility of the model was first established by validation using experimental temperature measurements. Subsequently, structural simulations were carried out under external load. The results of the simulations showed commendable agreement with the strain measurements performed using the developed technique.

Application of a multi-object tracking algorithm to investigate thermo-fluid dynamics of the melt pool during laser beam welding

Forster, Carola (1,5); Rothfelder, Richard (1,5); Krakhmalev, Pavel (2); Hummel, Marc (3); Spurk, Christoph (3); Beckmann, Felix (4); Schmidt, Michael (1,5)

1: FAU Erlangen-Nürnberg
2: Karlstad University, Sweden
3: RWTH Aachen University
4: Helmholtz-Zentrum Hereon
5: Erlangen Graduate School in Advanced Optical Technologies (SAOT)

16:50

Laser beam welding (LBW), as a non-contact process with short cycle times and small heat affected zone, is a key technology for automated metal fabrication. Despite its efficiency, the susceptibility of certain alloys to solidification cracks remains a significant challenge. These cracks emerge in the transition zone between liquid and solid phases during the solidification process. Thermo-fluid-dynamic processes within the melt pool play a crucial role in solidification crack formation during LBW, influencing heat distribution, mass transport, and, consequently, the microstructure and mechanical properties of the weld.

An in-depth exploration of thermo-fluid dynamics within the melt pool, contributes to an improved understanding of the correlations between process parameters and melt pool flow aiming to avoid solidification cracks. Therefore, in-situ process investigations were conducted at beamline P07 of PETRA III at the German Electron and Synchrotron Accelerator (DESY). 1.4404 stainless steel specimen containing an 5 wt. % of tungsten particles, serving as tracer, were additively manufactured using laser powder bed fusion. The tungsten particles are evenly distributed within the samples.

High-speed synchrotron X-ray imaging of the process zone allowed for detailed in-situ analyses. Leveraging the lower X-ray absorption coefficients of the base steel material compared to tungsten, the particles appeared as dark dots in the images. The experimental setup involved blind welds on the samples, where a portion of the sample was melted by the laser beam, forming a molten pool in the center while the edges remained intact. The uniform distribution of the particles in the sample means that the movement of the particles in the molten pool is overlaid by rigid particles located in the not melted edges of the sample. To enhance the observation and tracking of particle movement within the melt pool, the image contrast was optimized, and rigid particles were filtered out. The resulting images offered a visual representation of thermo-fluid dynamical flows during LBW, based on the movement of tracer particles. Analysis was performed using a data association algorithm for multi-object tracking.

The findings from this investigation provide valuable insights into the intricacies of thermo-fluid dynamics during LBW, offering a foundation for the advancement of numerical modeling and simulation tools in the field of laser beam welding.

Performance Analysis for the Free Surface Lattice Boltzmann Method for High Performance Computing

Plewinski, Jonas (1); Alt, Christoph (1); Rüde, Ulrich (1,2); Köstler, Harald (1,3)
1: FAU Erlangen-Nürnberg
2: CERFACS, France
3: Erlangen National High Performance Computing Center, Germany

17:10

waLBerla stands as a contemporary open-source framework for massively parallel multiphysics simulations, emphasizing its application in computational fluid dynamics (CFD). Utilizing the lattice Boltzmann method (LBM), it diverges from conventional Navier-Stokes solvers, enabling diverse CFD simulations. waLBerla boasts scalability on the foremost global clusters, owing to its meticulously crafted distributed data structures. Beyond pure CFD simulations, it facilitates the modeling of particle-laden flows and multiphase-flows. This is achieved through the employment of either the conservative Allen-Cahn phase-field LBM or the free surface LBM (FSLBM). The latter divides the simulation domain into three distinct phases—gas, fluid, and interface — where computation within the gas phase is disregarded. The interface delineates a one-cell-thick layer between the first two phases and yields computational challenges. The FSLBM has been validated physically but lacks a comprehensive performance analysis so far. This presentation aims to give an overview on node-level performance analysis, employing continuous benchmarking and scaling results on modern HPC clusters.

A microstructural thermoelastoplastic analysis of the mushy zone during laser beam welding

Hartwig, Philipp (1); Scheunemann, Lisa (2); Schröder, Jörg (1)
1: University of Duisburg-Essen
2: RPTU Kaiserslautern-Landau

17:30

As a modern method of contact free fusion, laser beam welding has gained importance in recent years. This is due to both the possibiliy of a high advance speed of the laser and low thermal distortion of the components compared to other welding processes, see [1]. These beneficial process properties follow from a focused laser, which thus results in a precise energy input. In addition, laser welding processes can be automated which makes the process more attractive for a wide range of applications, like the automotive industry, aerospace technology, shipbuilding, medical technology, the electrical industry or tool manufacturing, cf. [2]. Nevertheless, various influences, like the temperature gradient, the chemical composition or process parameters, can lead to so-called solidification cracks. Solidification cracks occur during solidification and develop from microcracks in the inside of the weld bead. They emerge to the surface with further cooling, see [3]. Furthermore, solidification cracks occur in the area of the mushy zone, which is located behind the melt pool. This is the area in which the material, after having been completely liquified, solidifies again. Accordingly, the zone lies exactly between the areas of complete solid phase and complete liquid phase. The mushy zone contains a dendritic morphology. Due to this structure, liquid phase inclusions may occur in some parts of the mushy zone. When these trapped areas solidify, no further liquid phase can follow and a negative pressure is created. The resulting stresses can then lead to solidification cracks. This contribution addresses the problem in a twofold way. In a first step, with a macroscopic view on the welded specimen, the mushy zone is identified through suitable heat source models, see [4] and [5]. Secondly, the evolving state of the dendritic microstructure is analyzed on a microscopic level, taking into account thermal as well as elastoplastic effects, in order to represent the inherent stress and strain states in the microstructure. These may be related to critical states leading to failure in the future.

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Efficient parallel finite element simulations of laser beam welding processes

Bevilacqua, Tommaso; Klawonn, Axel; Lanser, Martin; Wasiak, Adam
University of Cologne

17:50

Non-contact joining processes, such as laser beam welding, have become considerably more important in the course of the increasing degree of automation in industrial production. The laser has established itself as the preferred joining tool for metallic materials due to its non-contact processing, short cycle times and small heat-affected zones. However, a problem with this process is the occurrence of solidification cracks, which frequently occur when using materials that have a pronounced melting interval. This happens due to the high cooling rate inherent in the process that can lead to a residual melt oversaturated with certain alloy elements. Consequently to the fast shrinkage of the mushy zone, the joint gap that has to be covered by the melt widens steadily and can no longer be closed by the very slow-solidifying residual melt, resulting in a solidification crack.
A quantitative understanding of the development mechanisms of initial solidification cracks and their correlation to process parameters is indispensable for the development and improvement of the laser beam welding process and in the focus of the DFG research group 5134 "Solidification Cracks During Laser Beam Welding - High Performance Computing for High Performance Processing".
As a further step on the way of a quantitative process understanding, we here present large time-dynamic and HPC-supported finite element simulation of the mechanical and thermal stresses of thermoelastic laser beam welding problems using realistic process parameters and a high resolution. To obtain efficient and highly parallel scalable simulations, we use highly scalable and robust domain decomposition solvers.

Efficient Simulation Strategy to Investigate a PTW Safety Concept

Fehr, Jörg; Maier, Steffen
University of Stuttgart

18:10

Accidents involving powered two-wheelers (PTW) are complex events whose outcome depends on many factors. A violent ejection of the rider from the motorcycle is a very likely accident outcome. As a result of an impact against another road user, the road or roadside objects, the rider often suffers multiple serious injuries or even death. A novel restraint concept aims to solve this problem of insufficient passive safety for motorcyclists without compromising the advantages of a PTW as a compact means of transport, such as good all-round visibility and manoeuvrability, and without losing its unique driving characteristics. The innovative idea proposes that in the event of a crash impact, the rider is restrained by thigh belts, multiple airbags and leg impact protectors on the motorcycle. The objective of this work is to computationally model, simulate and investigate the proposed safety concept. The main research questions are: Is being restrained on a motorcycle safer than being subjected to the intrinsic unpredictability of a conventional motorcycle accident? What virtual models and numerical methods allow us to answer this?

The modelling and simulation strategy, targeting a time- and cost-efficient design and investigation of the concept, combines several individual development tasks in a methodology consisting of three successive virtual development stages with continuously increasing levels of detail and expected fidelity in multi-body and finite element simulation environments. For robust design, available numerical models of crash-test dummies and advanced human models are used. The vehicle and body substitute models are simulated in recommended representative crash scenarios and evaluated in kinematic, kinetic, and energy-based analyses, as well as with respect to a wide range of whole-body biomechanical injury criteria.

The results show what is possible with a fully virtual concept study. It is an efficient and effective simulation strategy that exploits the individual advantages of the different simulation models to predict the accident behaviour of the motorcycle, its passive safety systems, and different riders. The simulations show a guided and controlled trajectory and deceleration of the rider, resulting in less critical biomechanical loads compared to an impact with a conventional motorcycle. The combination of multiple passive safety systems shows great promise in positively influencing accident behaviour and mitigating accident consequences. The study is the first step towards a holistic evaluation of the innovative idea but its modelling still needs to include many more possible accident types to rule out harmful effects in beyond-design-basis scenarios.

S07.03: Laser beam welding

Date: March 20, 2024 08:30–09:30
Room: G16/215
Chair(s): Scheunemann, Lisa
Schneider, Daniel

Domain decomposition approaches for the saddle point problem of thermoelasticity

Bevilacqua, Tommaso; Klawonn, Axel; Lanser, Martin; Wasiak, Adam 08:30
University of Cologne

Non-contact joining processes, such as laser beam welding, have become considerably more important in the course of the increasing degree of automation in industrial production. The laser has established itself as the preferred joining tool for metallic materials due to its non-contact processing, short cycle times and small heat-affected zones. However, a problem with this process is the occurrence of solidification cracks, which frequently occur when using materials that have a pronounced melting interval. This happens due to the high cooling rate inherent in the process that can lead to a residual melt oversaturated with certain alloy elements. Consequently to the fast shrinkage of the mushy zone, the joint gap that has to be covered by the melt widens steadily and can no longer be closed by the very slow-solidifying residual melt, resulting in a solidification crack.
A quantitative understanding of the development mechanisms of initial solidification cracks and their correlation to process parameters is indispensable for the development and improvement of the laser beam welding process and in the focus of the DFG research group 5134 ”Solidification Cracks During Laser Beam Welding - High Performance Computing for High Performance Processing”.
As a further step towards the simulations of solidification cracks during laser beam welding, we consider multiple formulations of a thermoelasticity problem suitable for large temperature changes. After space discretization using the finite element method, we find that a nonsymmetric and perturbed saddle point problem must be solved in every time step. To ensure a robust and scalable iterative solution, different two-level domain decomposition methods are employed and compared with respect to robustness and numerical scalability. We additionally present the current state of the stability analysis in the framework of generalized saddle point problems.

CALPHAD-based thermodynamic modelling and phase field simulations of dendritic solidification in austenitic stainless steel

Umar, Muhammad (1,2); Schneider, Daniel (2); Nestler, Britta (1,2) 08:50
1: Karlsruhe University of Applied Sciences
2: Karlsruhe Institute of Technology

The austenitic stainless steel (X5CrNi18-10) is the most commonly used chrome-nickel steel, due to its good processing properties, visually appealing appearance and high corrosion resistance. However, it faces the challenge of hot cracking during post-laser-beam-welding dendritic solidification. Dendritic growth is a common phenomenon during the solidification of alloys, which significantly impacts the final microstructure and mechanical properties, whose complete understanding is still needed. The goal of this research is to fill this gap by looking at various aspects influenced by process-specific extreme thermal conditions at the microscale. Firstly, the objective is an accurate near-equilibrium thermodynamic modelling of quaternary (Fe-C-Cr-Ni) configuration using CALculation of PHAse Diagrams

(CALPHAD) database. It is then used to gain an understanding of the micro-segregation behaviour of alloying elements and resulting dendritic morphological parameters based on the local thermal conditions of the weld pool. For this purpose, a multi-component and multi-phase field approach is used in grand chemical potential-based phase field simulations. Based on the CALPHAD-fitted Gibbs energy functions, phase-field simulations are performed to observe similar dendritic/cellular solidification behaviour. The microstructure evolution influenced by local conditions such as thermal gradient and welding velocity at steady-state conditions is analyzed after theoretical validation of simulation results. It is observed that, apart from global processing conditions, local conditions are also important to consider. For instance, the morphology changes from columnar-dendritic to cellular moving from centerline to the fusion-line adjacent to the weld pool. Similarly, the micro-segregation changes so that the centerline becomes more prone to residual liquid pockets and hence microstructural defects. By analyzing the solidification microstructure, other valuable insights into the solidification kinetics and the influence of process parameters on dendritic growth are obtained. Further systematic analysis of these aspects from 2D and 3D simulations using the research data infrastructure Kadi4Mat for result generation, data analysis, storage and sharing capabilities yields interesting results on correlations of material and processing parameters. This comprehensive study along with mechanical contribution during solidification can help to understand the effect of process-related variables such as the temperature gradient, the welding speed and the heat input on the susceptibility to crack formation at the dendrite, grain/phase boundaries in the heat-affected zone and in the re-solidified weld seam.

Insights from Sustainable Data Management in Investigating Solidification Crack Formation

Janki, Atin 09:10
Karlsruhe Institute of Technology

In the realm of natural sciences and engineering, the surge in experimental and simulation data has underscored the pivotal role of adept digital research data and software management. This is particularly pronounced in the intricate domain of materials science, where the exploration of novel materials has intensified the complexity of research endeavors. The escalating volume of data mandates a paradigm shift in analysis methodologies to extract meaningful insights. To navigate this data deluge effectively, a structured approach to the storage of research data and associated metadata becomes imperative.

Motivated by the imperative to harness the full potential of burgeoning data, this paper delves into the intersection of coupled problems and sustainable data management in the context of investigating solidification crack formation during laser beam welding. We introduce Kadi4Mat, a Research-Data Management tool, and elucidate its role in storing and managing data according to FAIR principles. The focal point is on seamlessly accommodating the needs of researchers throughout the research lifecycle — from the inception or utilization of simulation software, structured data storage, exchange for analysis, to the eventual publication of findings. This infrastructure is envisioned to transcend geographical and institutional boundaries, fostering both centralized and decentralized, as well as internal and public use.

Our methodology also involves creating workflows within Kadi4Mat to automate various tasks, offer data manipulation and visualization; while ensuring efficient data coupling amongst data from various research groups. Drawing parallels between coupled problems in materials science and the challenges of managing diverse research data, we demonstrate how Kadi4Mat acts as a multi-field solution, seamlessly integrating interdisciplinary research data for the problem of the formation of solidification cracks in laser beam welding on a cross-scale and multi-physical basis. Our results highlight the benefits of structured data in Kadi4Mat, enhancing research outcomes and paving the way

for sustainable data management practices in coupled problems. Through a comprehensive discussion, we highlight the broader implications of our approach for materials science including improved quality of recorded data, speed-up data exchange and ways to extract meaningful insights from it.

S07.04: Phase-field models, Porous media

Date: March 20, 2024 14:00–16:00
Room: G16/215
Chair(s): Jänicke, Ralf
Ricken, Tim

Framework for an electro-chemo-mechanical multi-component multi-phase-field corrosion model

Dittmann, Jan; Wulfinghoff, Stephan 14:00
Kiel University

We present the framework for an electro-chemo-mechanical model for multi-component corrosion processes. The model is based on the framework for gradient extended standard dissipative solids and couples diffusion, chemical reaction, phase transformations, mechanical stresses, electrical fields and currents. The driving force for diffusion is given by the gradient of the electrochemical potential. Phase transformation and phase boundary movement is described by the Allen-Cahn equation in combination with a constrained double obstacle potential. To shift the constraint of the phase field parameter $\xi \in [0, 1]$ from the nodes to the Gauss points, the model makes use of the micromorphic approach. The model is designed to describe the formation, growth and dissolution of a corrosion layer on a material in a corrosive medium. Since the application of electrical fields and currents can be used to reverse the process it is also suitable to model certain battery processes.

A combined explicit-implicit approach for robust finite cell simulations of phase field fracture

Hosseini, Seyed Farhad; Gorji, Mahan; Sartorti, Roman; Radtke, Lars; Düster, Alexander 14:20
Hamburg University of Technology

In the phase field simulation of brittle fracture, we usually face two fully different convergence behaviours of the staggered solution approach: almost linear and fast converging load steps as well as highly non-linear and very slowly converging ones. The reason for this non-linearity comes from physical concepts like crack initiation/propagation at those critical load steps. Convergence at these critical load steps sometimes needs very high number of staggered iterations, sometimes as high as 1000. In finite cell simulations with complicated geometries, on one hand we cannot afford such high number of iterations and on the other hand, there is no guarantee to converge. Also in some cases, convergence curves shows a zig-zag behaviour which means that higher number of iterations does not necessarily mean higher accuracy. Also this non-monotonic convergence cannot be used for any prediction-correction and acceleration approaches. Addressing this problem, we propose a combined explicit-implicit approach to take the advantage of both techniques. The proposed method is implicit as long as the maximum number of staggered iterations has not been reached, otherwise, the current unconverged load step will be restarted and replaced by explicit load steps. The current implicit-failed load step then is subdivided into as much as possible explicit load steps. Using this technique, the highly non-linear part of the global load-displacement curves can be bypassed. The embedded technique will strongly increase the robustness of simulation. The effectiveness of the current method will be shown in some benchmark as well as practical examples and the effect of important model parameters will be discussed.

A Finite Element Approach to Multiphysical Problems in Poroelasticity

Reiff, Pit; Betsch, Peter
Karlsruhe Institute of Technology

14:40

In this talk, we will investigate porous media consisting of solid skeletons and a fluid phase within the pores. This is motivated by drying techniques, where a constant electric field is applied to masonry with the goal of reducing the moisture content within the walls.

Historically, the basics of poroelasticity have been established by Terzaghi and Biot, whose equations are the starting blocks of any kind of multiphysical modeling within porous media. Those equations consist of the momentum balance for the linear elastic (solid) continuum and the mass balance of the pore fluid. The resulting equations can be extended to partially saturated media and coupled with other fields like electrokinetics, ion transport and heat transfer. This enables the construction of finite element formulations that are able to consider the necessary mechanisms for practical applications, like the model problem of electroosmotic drying of building walls.

The prediction of such complex multiphysical phenomena requires reliable numerical methods. Therefore, after giving an (short) overview of the governing equations, we will present a solution strategy based on the Finite Element Method (FEM). This will enable the physically correct treatment of the coupled problem at hand.

Dual-phase field models for immiscible fluid flow through fractured unsaturated porous media

Peters, Sven (1); Heider, Yousef (2); Markert, Bernd (1)
1: RWTH Aachen University
2: Leibniz University Hannover

15:20

The immiscible multiphase fluid flow in intact and fractured porous media is relevant to numerous engineering sectors, including industrial processes, geo-engineering, and civil engineering. These encompass crucial applications that pose significant challenges in modeling, such as carbon dioxide (CO2) storage in underground reservoirs, contaminant transport, and desiccation-induced hydraulic fracturing in unsaturated soils [1]. In this work, a macroscopic framework is developed to describe the transport of immiscible and multiphase fluids in intact and fractured porous materials. The modeling approach utilizes the embedding of two phase-field models within the continuum Theory of Porous Media (TPM) [2].

To describe the flow through unsaturated porous materials, an extension of Darcy's law by a Cahn-Hilliard (CH) phase field model (PFM) [3] is proposed. This Darcy-CH-PFM approach is not only able to capture the fluid-fluid interaction but also able to include an additional macroscopic capillary pressure, which is formulated as a function of the phase-field parameter. The sharp crack topology in the fractured regions is approximated with another phase-field method that forms a diffusive transition zone across the crack edges of the deformable porous material. For the solid matrix, we consider a small strain assumption with a heterogeneous distribution of the permeability parameter. The inclusion of heterogeneity allows for a more realistic modeling of crack propagation and fluid-fluid interaction. For the numerical framework, the coupled system of differential-algebraic equations (DAE) is solved by the Finite Element Method (FEM), which is implemented in the open-source FeniCSx Project. In this, suitable stabilization techniques are also discussed.

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Non-intrusive inference of digital twins from conjugate, multiphase, porous media models to enable autonomous processes

Kannapinn, Maximilian; Schäfer, Michael; Weeger, Oliver 15:40
TU Darmstadt

A digital twin is a virtual representation that accurately replicates its physical counterpart, fostering bi-directional real-time data exchange throughout the entire process lifecycle. Traditionally, experts in the design phase leverage simulation and data science technologies for exploring various what-if scenarios. In contrast, digital twins embody an ambitious initiative to extend simulation insights to operational processes, empowering them to make autonomous, well-informed decisions [2].

Our proposed computational framework facilitates the automated extraction of digital twins from existing coupled simulation models. Notably designed for seamless integration within the industry, this framework found its first practical applications in deriving digital twins for autonomous thermal food processing [1] and in additive manufacturing. To streamline these processes, we introduce TwinLab, a comprehensive software suite that automates simulation model handling, training data selection, reduced-order model derivation, and digital-twin-based control techniques, all integrated into a single framework.

The pursuit of utmost accuracy in digital twins necessitates the creation of sophisticated multi-physical simulation models to establish a robust data foundation. To enhance the understanding of the product-process interrelationship, we propose a novel approach that couples porous media food processing models with non-isothermal flow and thermal radiation within a convection oven. This approach reveals substantial differences, surpassing the accuracy of traditional transfer-coefficient-based models found in the literature. For instance, a conjugate simulation of a food item exhibits local temperature variations up to E_{max} = 48 K (30.6% relative error), and water saturations differ by E_{rel} = 60%.

The provision of real-time replication highlights a critical challenge faced by modern computational engineering. As the complexity and computational cost of multi-physical simulation models increase, computing power struggles to keep pace, rendering real-time simulations, especially on low-end processors, unfeasible. Our work addresses this challenge by showcasing how digital twins can be efficiently trained with just one-to-two training data sets extracted from multi-physical simulation models. We propose an effective design of experiments that aids in selecting training data, ensuring a low test error of the twin on representative test data. Notably, the root-mean-square errors for the best twins range from 0.30 to 0.83 K, and the time series' relative error of 0.18–0.49% surpasses the validation errors of the employed processing models.

The efficiency gains achieved in our digital twin implementation are significant, with attainable speed-ups compared to real time reaching approximately Sp 3.6 × 1E4. Characteristic solution times of one-tenth of a second demonstrate computational efficiency without imposing a noticeable cost on a single-core processor. Importantly, field data with 4649 points in space and one hour of real-time processing outputs can be predicted within less than half a second, showcasing the practical viability of our proposed digital twin framework.

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S07.05: Porous media, Thermomechanical problems

Date: March 20, 2024 16:30–18:30
Room: G16/215
Chair(s): Radtke, Lars
Hosseini, Seyed Farhad

Modeling coupled damage processes in porous media across the scales

Bharali, Ritukesh (2); Larsson, Fredrik (2); Jänicke, Ralf (1) 16:30
1: TU Braunschweig
2: Chalmers University of Technology, Sweden

Material properties and damage evolution in engineering structures are controlled by coupled multifield processes on various length and time scales that might ultimately result in the collapse of the entire structure. Often, such deterioration processes are driven by transport of a liquid phase or further mobile species such as e.g. Chloride ions in concrete [1] through pore networks or along highly conductive fractures embedded in a solid phase.

In this contribution, we will discuss concepts for 3D-imaging of coupled transport and crack propagation processes over time using X-Ray Computed Tomography with in-situ testing. 1. We will present concepts to model coupled degradation processes in porous media. Hereby, we employ a micromorphic phase-field model to describe crack initiation and propagation where the conventional energy functional pertaining to the linear elastic single phase media is extended towards two-phase (partially) saturated porous media. The micromorphic model retains the phase-field fracture length-scale, however, with a new variable for regularization. The phase-field is, therefore, transformed into a local quantity (evaluated at integration points), which enables fracture irreversibility enforcement with system-level precision.

Finally, we will transfer effective material properties to a larger scale by means of Variationally Consistent Computational Homogenization [2, 3]. The presentation will be concluded with numerical studies.

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Numerically efficient solution methods in highly nonlinear variational thermoinelasticity

Goldbeck, Hauke; Wulfinghoff, Stephan 16:50
Kiel University

We present a modified Newton scheme applied to a thermomechanical shape memory alloy model, which improves the convergence. Key feature of the model, which is a modified version of the model by Sedlák et al. 2012, is its capability to accurately model the shape memory effect, as well as the superelastic behavior by a thermomechanical potential, compare with Sielenkämper & Wulfinghoff 2022. The variation of this potential yields the energy balance, the linear momentum balance and the evolution equations of the internal variables. Yield and transformation criteria are derived form the corresponding dual dissipation potential. In order to improve the convergence of the thermomechanical model the Newton scheme is adapted using a line search approach. Therefore, the residuum

of the convex thermomechanical potential is linearized. The step size of each Newton step is adapted such that the local minimum of each step is approximated as starting point for the following Newton step. This approach improves the numerical robustness of the Newton scheme.

Implementation of a thermomechanically coupled constitutive model for single-crystalline SMA based on an Augmented Lagrangian formulation

Löps, Paul; Prüger, Stefan; von Oertzen, Vincent; Kiefer, Bjoern 17:10
TU Bergakademie Freiberg

Shape memory alloys (SMA) can undergo reversible solid state phase transformations from the high temperature austenitic phase to the low temperature martensitic phase, which is the origin of their unique thermoelastic properties. More specifically, at the single crystal scale these mechanisms occur on discrete transformation systems dictated by the crystal symmetry. Even in the fully transformed, twinned martensitic state, a reselection of martensite variants is observed upon deformation, which is commonly referred to as variant reorientation. During the last decade, several constitutive models that describe these experimentally confirmed phenomena - accounting also for anisotropy and finite deformations - have been proposed. However, the robust determination of the set of active transformation systems is still challenging, particularly in the rate-independent case, for which the problem is ill-posed.

Recently, an Augmented Lagrangian formulation of the principle of maximum dissipation has been successfully applied in a constitutive model of single crystal plasticity [S. Prueger, B. Kiefer, Int. J. Mech. Sci., 180, pp. 105740, 2020], thus leading to a robust determination of the set of active slip systems.

Here, this framework is extended to incorporate bound constraints on the martensite variant volume fractions, whereby the reformulation and implementation of a constitutive model for single crystal NiTi-SMA, described in [L. Anand, M.E. Gurtin, J. Mech. Phys. Solids, 51(6), pp. 1015-1058, 2003], is adopted.

It is demonstrated that the implemented, thermomechanically coupled model allows for the description of variant reorientation and the one-way shape memory effect as well as self-heating due to the latent heat of transformation.

The robustness of the proposed formulation is verified by representative examples at the material point level and in three-dimensional finite element simulations of single crystal tension and compression specimens.

Thermomechanically coupled finite element formulation for strain-induced crystallization

Tang, Xuefeng (1); Poudel, Rabin (1); Itskov, Mikhail (1); Jabareen, Mahmood (2); Khiêm, Vu Ngoc (1) 17:30
1: RWTH Aachen University
2: Technion – Israel Institute of Technology

In this contribution, a thermomechanically coupled finite element formulation for strain-induced crystallization of natural rubbers is presented. The formulation is based on our theoretical derivations [1,2] in which deformation induces both phase transition and internal heat transfer after the onset of crystallization. A mixed finite element formulation is then developed for natural rubbers, taking into account their nearly incompressible behavior. The robustness of the proposed formulation is demonstrated in several benchmark examples, while its accuracy is confirmed by validation with infrared thermography-based quantitative surface calorimetry measurements available in the literature.

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Thermomechanical analysis of strain recovery in shape memory alloys under variable non-isothermal conditions

Descher, Stefan (1); Krooß, Philipp (2); Ewald, Felix (2); Kuhl, Detlef (1)
1: Institute of Structural Mechanics, University of Kassel
2: Institute of Materials Engineering, Metallic Materials, University of Kassel

17:50

A major reason for the application of shape memory alloys (SMAs) is to make use of the one-way effect. It allows recovering plastic strains that are mechanically brought into the material by thermal activation due to heating. The underlying process is a phase transformation from a martensitic phase (M) to an austenitic phase (A) that occurs in a certain temperature range. It resets the change of microstructure that was introduced mechanically, and therefore, e.g., allows making use of restoring strains. A popular application of SMAs are actuators, often found in aviation [1] and automotive industry, or as smart reinforcements in novel materials of civil engineering, see [2].

As found out in the preceding thermodynamic studies of the present work in [3], latent heat effects play a key role in this activation process. The heat sink caused by the M-A phase transformation during activation causes an interface of transformation to move through the material. This highly depends on the local heating rate, that is reached during activation. To further study this behavior, in the present work, mechanical coupling is realized. Studies are carried out for a characteristic non-isothermal tension test, as it is performed to record stress-strain-temperature curves as presented in [1]. For this purpose, the M-A phase transformation is described by a phenomenological evolution equation, which is solved together with the Cauchy-Fourier equations using the Finite Element Method.

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Basic problems of steady vibrations in the coupled theory of thermoelastic nanomaterials with triple porosity

Svanadze, Merab
Ilia State University, Georgia

18:10

In this work, the coupled linear theory of thermoelastic nanomaterials with three levels of pores (macro-, meso- and micropores) is considered. In this theory the combination of Darcy's law and the volume fraction concept for triple porosity materials is provided. The basic internal and external boundary value problems (BVPs) of steady vibrations are formulated. Then, the uniqueness theorems are proved using Green's identities. The formula of integral representation of regular vectors is obtained. The surface (single-layer and double-layer) and volume potentials are introduced and their basic properties are established. Some useful singular integral operators are defined for which Noether's theorems are valid. The symbolic determinants and indexes of these operators are calculated explicitly. The BVPs of steady vibrations are reduced to the equivalent singular integral equations. Finally, with the help of the potential method and the theory of the singular integral equations, we prove the existence theorems for classical solutions of the aforementioned BVPs.

Acknowledgments. This work was supported by Shota Rustaveli National Science Foundation of Georgia (SRNSFG) [Project # STEM-22-557].

S07.06: Chemo-/thermo-/hygro-/electro/-mechanical coupling

Date: March 21, 2024 08:30–10:30
Room: G16/215
Chair(s): Hellebrand, Sonja
Brands, Dominik

On the effects of coupling in a thermo-chemo-mechanically model

Gisy, Johannes; Dyck, Alexander; Böhlke, Thomas 08:30
Karlsruhe Institute of Technology

In emerging technologies, it is important to understand diffusion driven motions of species in solids, for example hydrogen diffusion in metals and moisture diffusion in polymers [1]. Besides these examples where diffusion may occurs depending on the environmental conditions, there are other applications, i.e., batteries [2] and solid oxide fuel cells (SOCFs), where the motion of the species is indispensable for the working principle. In the first case, it is important to predict the influence of specific environmental conditions on the solid material, whereas the limits of structural stability and life-time at high efficiency is the goal in the second case. Thus, robust numerical models, which reproduce the relevant physical phenomena, are needed [3].

Within this talk, a fully coupled thermo-chemo-mechanical model is presented. The model combines the three fields displacement, chemical potential and temperature, and is shown to be thermodynamically consistent [4]. The mechanical behavior is described in a small deformation setting. The chemical behavior is built up on a standard diffusion model and the thermal behavior is described by a heat conduction model of Fourier type. Due to the coupling of three fields, the implementation enables to study rather different coupling scenarios. In the talk, we discuss several weak and strong coupling cases.

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Thermo- and chemo-elastic beam modeling and simulation with isogeometric collocation methods

Alzate Cobo, Juan Camilo; Weeger, Oliver 08:50
TU Darmstadt

The shift towards more sustainable energy sources allows for lattice structures to play an emergent role in the design of future generations of energy storage and conversion devices, such as Li-ion batteries and thermoelectric generators. Particularly, three-dimensional electrode architectures have the potential to provide shorter ion-diffusion paths due to the greater surface-to-volume ratios of the active electrode material. Thus, the power density of batteries can be improved, which leads to shorter charging times. Nevertheless, the modeling and simulation of lattices structures (let alone their optimization) with commonly used methods, such as continuum finite elements, is computationally expensive. A way to mitigate this adversity is the use of beam theories. However, an efficient numerical scheme for the modeling and simulation of 3D beams that allows for large volumetric strain, induced primarily by Li-ion diffusion, has not been found in the literature. This contribution aims to provide essential steps in this direction.

For the Cosserat beam, a mixed isogeometric collocation method (IGA-C) that alleviates locking phenomena has already been developed and validated. In this contribution, this model is further enhanced to incorporate axial and radial strains, both small and large, that result from the beam's interaction with a temperature or a concentration field. Additionally, the elastic beam quantities, i.e., the stress and strain resultants, are thoroughly derived from principles consistent with 3D continuum mechanics. The latter is achieved following a multiplicative split of the deformation gradient. Moreover, the coupling of the mechanical with the thermal/chemical system is realized through a staggered

scheme, where the diffusion equation is also solved following an IGA-C approach. Assuming rotational symmetry of the temperature or the concentration field, the diffusion equation is reduced to a 2D problem, thus improving the overall computational effort while retaining reliable results.

The novelty of the presented method is twofold. First, it relates beam theory, and consequently small elastic strains, with large swelling deformation stemming from diffusion phenomena. Second, it also provides insight into the implementation of IGA-C for solving diffusion equations subject to large deformations. Ultimately, the current model represents the starting point for the coupling between thermo- and chemo-mechanics, beam theory, and IGA-C.

Hygro-thermo-mechanical modelling of frozen ground and shotcrete interaction during tunneling excavation

Williams Moises, Rodolfo Javier; Meschke, Günther 09:10
Ruhr University Bochum

Artificial ground freezing is used for ground improvement in tunneling. Ground freezing is often applied to control water seepage and to increase the bearing capacity of the ground. Ground freezing is commonly used to stabilize the ground before the excavation of cross passages in tunneling. During the construction of the cross passages, the frozen ground is excavated and the tunnel is supported immediately by shotcrete shells. In this contribution, we present a computational framework for the modelling of the thermo-hygro-mechanical interaction of frozen ground and shotcrete during cross-passage construction. The computational framework consists of a three-phase thermo-hygro-mechanical finite element model for the modelling of soil freezing based on [1] and a three-phase thermo-mechanical finite element model for shotcrete based on [2]. This framework considers the evolution of the stiffness, strength, and creep properties and the hysteresis effects during freezing-thawing of the ground in conjunction with the shotcrete hydration and creep deformation. Finally, we present a numerical case study of this tunneling problem which is modelled in two stages: the first stage involves the modelling of a freezing phase imposed by the soil freezing and the second stage involves the tunnel excavation, the shotcrete installation with its internal hydration heat generation and the evolution of the hydration dependent primary creep deformations.

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Coupled chemo-electro-mechanical model for galvanic corrosion in clinched components

Harzheim, Sven; Chen, Chin; Hofmann, Martin; Wallmersperger, Thomas 09:30
TU Dresden

Mechanical clinching is a frequently used joining method for technical components. Weak points in technical components are often these joints. Here, corrosion and fatigue are decisive influencing factors for the assessment of the service life. Corrosion generally leads to material deterioration and thus to premature failure of the joints. Under certain circumstances, however, corrosion can lead to an increased fatigue life of clinched joints. While this effect has not yet been fully understood, the present work provides a possible explanation and a modeling approach to predict the fatigue life of pre-corroded clinched joints.

The increased fatigue life is observed when the clinched components are briefly (up to three weeks) exposed to a salt spray environment. During this time, a small layer of corrosion products protrudes from the metal surface and fills the gaps between the joined sheets. Due to the increased contact area, the mechanical stress in the joint decreases, resulting in an improved fatigue performance.

Although there are a variety of corrosion phenomena, e.g. pitting corrosion, intergranular and transgranular corrosion as well as galvanic corrosion, experimental studies indicate that galvanic corrosion is the main contributor of this effect.

In the present work, a coupled electro-chemo-mechanical corrosion model is presented, which mathematically describes (i) mechanical loading of the clinched joints, (ii) production of corrosion products due to galvanic corrosion and (iii) metal dissolution simultaneously.

Implementation of a Finite-Element Framework Coupling Chemo-Mechanics and the Non-Local Gurson-Tvergaard-Needleman Model

Patil, Siddhi Avinash; Prüger, Stefan; Roth, Stephan; Seupel, Andreas; Kiefer, Bjoern 09:50
TU Bergakademie Freiberg

Hydrogen embrittlement in ductile metals, such as steel, is a significant concern, for instance, in the safety assessment of existing pipeline infrastructure intended for hydrogen transport. The ductile damage mechanism in steels is characterized by the nucleation, growth, and coalescence of microvoids, which is further enhanced by the presence of hydrogen. This leads to material damage and premature failure in components. Mechanisms contributing to hydrogen-induced reduction of strength in steels include hydrogen-enhanced decohesion (*HEDE*), hydrogen-enhanced local plasticity (*HELP*), and hydrogen-enhanced strain-induced vacancies (*HESIV*), see [1]. The HEDE mechanism leads to a principal stress-controlled brittle failure mode. Conversely, the HELP and the HESIV mechanisms, which are dominated by plastic deformation, alter the ductile damage behavior as they lead to accelerated void growth and coalescence. Furthermore, interstitial diffusion of hydrogen leading to lattice expansion, commonly referred to as swelling, also contributes to hydrogen-induced embrittlement. Hydrogen embrittlement is therefore a stress-diffusion process that involves chemo-mechanical coupling, where hydrogen atoms primarily diffuse toward areas with high hydrostatic stress. In this regard, we propose a framework using the finite-element method and combining coupled chemo-mechanics and the well-known non-local Gurson-Tvergaard-Needleman (GTN) damage model [2, 3]. The framework is based on mixed rate-type potentials, as introduced in [4], that account for the influence of hydrogen concentration on the damage behavior. An additional dependence of the fracture strain and evolution of the void volume fraction on hydrogen is included, as suggested in [1]. A comparison of the fully-coupled model to simplified versions is conducted to individually assess the role of hydrogen concentration on damage evolution and the stress state on diffusion.

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S07.07: Magnetic/ferrorelectric/dielectric/piezoelectric materials

Date: March 21, 2024 14:00–16:00
Room: G16/215
Chair(s): Graf, Matthias
Hackl, Klaus

Domain wall dynamics in cubic magnetostrictive materials subject to Rashba effect and non-linear dissipation

Maity, Sumit (1); Dolui, Sarabindu (1); Dwivedi, Sharad (1); Consolo, Giancarlo (2)
1: National Institute of Technology Andhra Pradesh, India
2: University of Messina, Italy

14:00

This work focuses on the analytical investigation of domain wall motion occurring along the major axis of a thin magnetostrictive nanostrip perfectly arranged on the top of a thick piezoelectric actuator. The motion is driven by magnetic fields, spin-polarized currents, and spin-orbit torque effects and takes place in cubic magnetostrictive materials characterized by a nonlinear dissipation. The main aim is to describe how magnetoelasticity, Rashba field, dry-friction, chemical composition, and crystal symmetry affect the steady and precessional dynamics of magnetic domain walls. In detail, it is here analytically inspected how the key features (threshold, breakdown, domain wall mobility, and propagation direction) can be effectively manipulated by the above contributions. Finally, the theoretical results are numerically illustrated for realistic materials, revealing a satisfying qualitative agreement with experimental observations.

Finite element based micromagnetic simulations of heterogeneous microstructres

Reichel, Maximilian; Schröder, Jörg
University of Duisburg-Essen

14:20

Cutting edge permanent magnetic materials such as neodymium-iron-boron (NdFeB) magnets play a crucial role in pushing the efficiency of power conversion devices, including wind turbines, sensors and electric motors to their limits, cf. [1]. Since they have the potential to strongly influence current technological and social challenges such as the reduction of carbon dioxide emissions, there is an increasing industrial and research driven interest in their enhancement. Although current state of the art magnets are very efficient, a wide range of improvements, as the general increase in performance, the exchange of environmentally critical elements by harmless substances as well as the reduction of their required production energy, is still possible. Here, microstructure engineering offers great potential by targeted influencing of the local structural compositions and thereby improving the magnetic properties. To support this process finite element based micromagnetic simulations can be a strong tool to numerically predict the magnetization distributions on fine scales. The FEM is characterized by a particularly flexible and not necessarily regular discretization, which is an advantage compared to other numerical methods for the discretization of heterogeneous microstructures, cf. [2]. The evolution of the magnetization vectors follows Gilbert's equation that merely permits movements on the unit sphere's surface, cf. [3]. This constraint is enforced via a condensed perturbed Lagrange multiplier, cf. [4].

Within this contribution high-resolution micromagnetic simulations of strongly heterogeneous magnetic microstructures are presented. Thereby, the focus remains on analyzing the influence of grain boundary layers and inhomogeneities within the bulk material that often act as weak spots enabling premature reversal.

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Fully-Coupled Finite Element Implementation of a Constitutive Model for Magnetic Shape Memory Alloys

Jeeja, Akshay Balachandran; El Khatib, Omar; Kiefer, Bjoern 14:40
TU Bergakademie Freiberg

Magnetic shape memory alloys (MSMAs) are intrinsically multiferroic, exhibiting both ferroelasticity and ferromagnetism when cooled below their respective phase transformation and Curie temperatures. They show strong magneto-mechanical coupling, inducing substantial shape changes and ability to regain their original shape under various loading conditions. These distinctive attributes have led to the exploitation of MSMAs in applications ranging from actuation and sensing to energy harvesting and smart structures. Extensive research has been conducted to develop models that can accurately describe the complex behavior of MSMAs, which includes hysteresis, non-linearity, and the dependence on stress and magnetic field levels. While numerous constitutive models have been formulated to describe the MSMA behavior, their practical utilization in commercial design applications necessitates their integration into finite element frameworks. The inhomogeneous distributions of the demagnetization field variables inside the MSMA specimen can only accurately be captured in such numerical simulations.
A micromagnetics-inspired variational framework is combined with a 3D constitutive model, that accounts for three different martensitic variants evolving in the MSMA microstructure, cf. [1,2]. A novel mixed finite element formulation is employed for the spatial resolution of magnetic and mechanical degrees of freedom, with the state variables characterizing the MSMA microstructure treated as global fields, see [3]. The model demonstrates its ability to predict characteristic magnetization curves. The volume-averaged strain and magnetization response curves for magnetic field-induced and stress-induced magnetic shape memory behavior are studied. The inhomogeneous nature of the strain and magnetization responses is carefully investigated. The influence of the model parameters and the magneto-mechanical field level dependence on MSMA response behavior is further assessed via detailed sensitivity analysis. The study also examines the model's capability to accurately represent intricate 3D loading scenarios, where all three variants may evolve simultaneously.

References

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Effect of nonlinear viscous dissipation on magnetic domain wall motion in transversely isotropic hexagonal magnetostrictive materials

Maity, Sumit 15:00
National Institute of Technology Andhra Pradesh, India

The prime focus of this study is to theoretically examine how the nonlinear viscous dissipation affects the strain-controlled magnetic domain wall motion in a transversely isotropic hexagonal crystal class of magnetostrictive nanostrip. The magnetostrictive nanostrip is assumed to be positioned atop a thick piezoelectric layer. We perform an analytical analysis through a mathematical framework that describes the motion of the domain walls in magnetostrictive nanostrip via the Extended Landau-Lifshitz-Gilbert Equation, which includes the external fields (magnetic and electric), mechanical strains via piezoelectric layer, and nonlinear viscous-dry fiction dissipations. We consider a mathematical tool such as the traveling wave method to derive the analytical expression of the key quantities like velocity, width, threshold, and Walker breakdown in the steady and precessional regimes. Moreover,

the nonlinear viscous mechanism causes the domain wall's velocity profile to become nonlinear. Next, we numerically illustrate the analytical results of domain wall velocity using realistic parameter values. This study is in qualitative agreement with recent observations.

Analytical and numerical investigations of Maxwell-stress-induced higher-order singularities in cracked dielectrics and piezoelectrics

Behlen, Lennart; Nickel, Felix; Wallenta, Daniel; Ricoeur, Andreas 15:20
University of Kassel

Linear elastic fracture mechanics deals with unbounded stresses at the tips of sharp cracks due to external loading by introducing stress intensity factors quantifying the characteristic square root singularity. In the process, higher-order singularities are basically discarded as they result in divergent mechanical energy of domains enclosing the crack tips. In fracture mechanics of dielectrics subjected to additional electric fields for the purpose of multifunctional applications, however, such higher-order singularities may naturally arise due to electrostatic action of force encompassing surface tractions as well as body forces and couples.

While microscopically these electric loads originate from the Lorentz force on point charges, macroscopically they are derived from the so-called Maxwell stress tensor, whose formulation in polarizable media is still being debated at present. A corresponding formulation of this tensor is commonly chosen from three established models according to either Minkowski, Einstein and Laub or Lorentz, each yielding dissimilar forces and couples.

Our work explores these singularities and draws conclusions with respect to the loading situation at the crack tip by means of analytical as well as numerical methods. On the one hand, analytical considerations are restricted to linear problems of anisotropic infinite dielectrics as they may be solved in closed form exploiting complex analysis and holomorphic potentials, respectively. Owing to the nonlinearity of the field equations including Maxwell stress, piezoelectrics exhibiting inherent constitutive coupling between mechanical and electrical state variables, on the other hand, are studied numerically employing the open-source code FEniCS.

Impact of inertial and nonlinear damping effects on the strain-induced domain wall motion in bilayer composite structure

Dolui, Sarabindu; Dwivedi, Sharad 15:40
National Institute of Technology Andhra Pradesh, India

This article analytically investigates the combined impact of inertial and nonlinear damping (viscous and dry friction) effects on the strain-controlled dynamic features of domain walls in an isotropic, linearly elastic hybrid bilayer piezoelectric-magnetostrictive composite structure. To be precise, we perform the analysis under the framework of the one-dimensional inertial Landau-Lifshitz-Gilbert equation, considering the influences of stresses induced by a piezoelectric actuator. By employing the classical traveling wave ansatz, this study explores how various factors, such as magnetostriction, magnetoelasticity, viscous, dry friction, and inertial damping effects, characterize the motion of the magnetic domain walls in both the steady-state and precessional dynamic regimes. The results exhibit valuable insights into how these key parameters can effectively modulate dynamic features such as domain wall width, velocity, mobility, threshold, and Walker breakdown limits. The obtained analytical results are further numerically illustrated for metallic and semiconductor ferromagnet, and a qualitative comparison with recent observations is also presented.

S07.08.1: Magnetic/ferrorelectric/dielectric/piezoelectric materials

Date: March 21, 2024 17:40–18:40
Room: G16/215
Chair(s): Reichel, Maximilian
Kiefer, Bjoern

A hybrid approach for ferroelectric continua combining the finite element method and an efficient scale bridging concept

Wakili, Reschad; Stephan, Lange; Andreas, Ricoeur 17:40
University of Kassel

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, 5]. 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 [4]. 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

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Material modeling of ferroelectric solids in presence of flexoelectricity

Kozinov, Sergey; Tannhäuser, Kevin 18:00
Ruhr University Bochum

Flexoelectricity refers to the advanced two-way interaction between strain gradients and electric fields, a phenomenon that becomes increasingly significant at smaller scales, making it a crucial factor in the development of high-precision micro- and nano-electromechanical systems, including sensors, actuators, and energy harvesting devices. The present study tackles the innovative challenge of modeling ferroelectric materials in presence of flexoelectricity. This issue can be approached from two perspectives: firstly, as an advancement in ferroelectric modeling by integrating higher-order electromechanical interactions, and secondly, as an extension of flexoelectric modeling within dielectric [1] and piezoelectric [2] structures to encompass nonlinear material behavior. This dual view offers a more comprehensive understanding of the interplay between ferroelectricity and flexoelectricity in complex material systems. The present study focuses on the development of the constitutive relations for the higher-order electromechanical coupling based on the micromechanical switching

model for ferroelectric polycrystals [3]. The corresponding numerical 3D implementation is carried out by further developing the recently presented collocation-based mixed FEM [1] and extending the ferroelectric switching model [4] with finite elements of higher order. The focus of the numerical simulations is on the alteration of the ferroelectric polarization and the strain hysteresis loops in the presence of flexoelectricity. The findings from this research are currently being compiled and refined for a manuscript, which is being prepared for submission [5].

References

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Numerical detection of shaft misalignments using a sensor-integrating jaw coupling

Menning, Johannes Dieter Martin; Ewert, Arthur; Prokopchuk, Artem; Schlecht, Berthold; Henke, E.-F. Markus; Wallmersperger, Thomas

TU Dresden

18:20

Shaft misalignments are one of the main causes of damage to couplings in machines, which can lead to machine downtimes if they are not recognized in time. During assembly of a machine, it is not always possible to perfectly align the shafts to each other. Elastic couplings are able to compensate such misalignments up to a certain degree. To detect whether a misalignment becomes critical, both a sensor-integrating jaw coupling and a first prototype were presented in [1]. In the teeth of the gear rim bore holes are drilled and dielectric elastomer sensor (DESs) are inserted. If the teeth deform during use of the coupling the DES will deform as well, leading to a change in capacitance, which can be detected. If the two shafts, which the coupling connects, are perfectly aligned to each other, each of the loaded teeth will deform uniformly. However, if there is a radial or angular misalignment, the deformation is different for each tooth, which can be determined with the help of the DESs. To demonstrate this effect, a finite element model is created and numerical simulations of the sensor-integrating jaw coupling are conducted. In this model, the hyper-viscoelastic material behavior of (i) the gear rim of the jaw coupling and (ii) the DES is taken into account. From the mechanical simulation the deformed state of the DES is obtained, which is used to compute the capacitance of the sensor.

With the results of the numerical simulations, a recurrent neural network model is trained on the measured capacitance of the DES to give predictions whether the misalignments are critical or not.

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S07.08.2: Fluid-structure interaction

Date: March 21, 2024 17:40–18:40
Room: G22/H2
Chair(s): Brands, Dominik
Hellebrand, Sonja

Experimental characterization of acoustic damping materials

Marter, Paul (1); Radtke, Lars (2); Eisenträger, Sascha (1); Düster, Alexander (2); Juhre, Daniel (1) 17:40
1: Otto von Guericke University Magdeburg
2: Hamburg University of Technology

Due to their ease of use and low cost, passive damping methods are a preferred means for the reduction of noise in many engineering applications. Foam materials, in particular, showing good acoustic damping properties, are often employed. The selection of suitable materials is usually carried out experimentally and can be very labor-intensive and time-consuming. For this reason, it is helpful to develop qualified numerical methods that can be used for material design and selection. Hence, foam materials must be characterized experimentally in order to enable a later comparison with vibroacoustic simulations. This contribution, therefore, aims at providing suitable parameters for the use in and the validation of numerical simulations.

Firstly, the microstructure of a foam specimen is captured by means of a CT scan. In addition to providing the geometry for the multi-physics simulations, this measurement is also used to determine characteristic foam features, e.g., the strut thickness and pore size distribution. In the second step, the frequency-dependent stiffness and damping properties of the material are determined by a special experimental set-up utilizing an electrodynamic shaker. Here, the dynamic system is approximated as a single-mass oscillator, which is sufficiently accurate and valid only at low frequencies. These properties will later be used in the numerical model to evaluate different parameter identification approaches. In the third and last step of the experimental campaign, measurements with an impedance tube are conducted to obtain the coefficient of absorption. This material parameter is particularly suitable for comparing experiments and simulations. Finally, the extent to which the results from the various experiments correlate is examined to provide a deeper understanding of the foam materials.

An automatic simulation pipeline for coupled simulations of acoustic damping materials

Radtke, Lars (1); Marter, Paul (2); Eisenträger, Sascha (2); Juhre, Daniel (2); Düster, Alexander (1) 18:00
1: Hamburg University of Technology
2: Otto von Guericke University Magdeburg

Foamed damping materials are widely used to reduce noise due to their comparably good acoustic damping properties. However, out of a large variety of these materials, a suitable one has to be identified for each application. This is a challenging process that is typically guided by experiments. While numerical simulations could support these experiments and reduce the effort to a great extent, no suitable discretization approach has yet been established that can fully capture the complex geometry of the foam. A fully resolved model is desirable in order to achieve reliable predictions that can then be used to establish homogenized models.
We present a monolithic coupling approach based on the finite cell method (FCM) [1]. The fluid and the structure domain are discretized by Cartesian grids and a space tree quadrature is employed to accurately capture the geometry. A voxel model obtained using a micro CT scanner provides the data needed to establish an inside-outside test. The interface is further triangulated in order to provide a basis for the integration of the coupling terms. Our simulation in the time domain makes use of explicit time marching schemes and is therefore limited by a critical time step size. This is known to be arbitrarily low for discretizations with the FCM containing cells with arbitrarily small support. As a remedy against this we make use of a novel eigenvalue stabilization technique [2] and IMEX time integration schemes [3].

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An approach simulating interacting solid, liquid and gas domains for dynamic seal applications

Graf, Matthias; Tobias, Lankenau
University of Applied Sciences Emden-Leer

18:20

In seal applications a solid elastic body (the seal) ensures the separation of a liquid (e.g. hydraulic oil in one chamber) from a gas (e.g. air in another chamber). In the case of a dynamic seal, the rod is moving and transportes a thin liquid film from the liquid chamber into the air chamber. The seal gap consists of a converging gap, a minimum distance between seal and rod and a diverging gap, where transported liquid detaches from the seal. Between the three states of matter (gas, liquid, gas) appear the following contact conditions: liquid-to-solid, gas-to-liquid and gas-to-solid. A classical fluid-structure-interaction is technically possible with limited effort, but is not sufficient to distinguish between the liquid and the gas. A solution can make use of the fact, that the liquid has significant dimensions only in the liquid chamber and is pressurized only there. There is a thin liquid film on the rod in the air chamber, but it has dimensions clearly lower than the air chamber and has the same pressure as the air. Therefore a simulation is possible with the "variable viscosity approach": Liquid and gas are modelled in one single fluid domain. Differences between liquid and gas are included by pressure-dependend fluid parameters, especially viscosity and density. The resulting violation of the mass balance is very small as the low mass flow through the seal lip is low. The presented approach allows to apply a fluid-structure simulation with special fluid properties to model a system with three states of matter. Advantages are a less complex model with less complex contat conditions and a reduced simulation time.

S07.09.1: Magnetic/ferrorelectric/dielectric/piezoelectric materials, Coupled flow problems

Date: March 22, 2024 08:30–10:30
Room: G16/215
Chair(s): Hartmann, Stefan
Schröder, Jörg

On the influence of the microstructure model on multiscale bone simulations

Blaszczyk, Mischa; Hackl, Klaus
Ruhr University Bochum

08:30

Osteoporosis is the most common bone disease in the world, affecting one in three women and one in five men over the age of fifty. The disease is characterized by weakening the bone, increasing the likelihood of fractures. Numerical simulations are an important tool for better understanding the workings of human bones, thus possibly opening the way for new diagnostic methods such as sonography. For this purpose, we developed a two-scale bone model that considers mechanical, electric and magnetic effects [1-3]. We use the finite element square method (FE2) to connect the scales. In this talk, we investigate the influence of the used microstructure model in detail. We created different representative volume elements (RVEs), which are e.g. anisotropic, differ in shape or mesh resolution, or are randomly rotated. In addition, we consider the use of different shape functions in the finite element calculation. We compare our findings with previous results, which were obtained using only regular RVEs. We investigate the extent, to which the microscale results and the overall macroscale simulation results are affected by the choice of the RVE.

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Efficient and Accurate Numerical Simulation of Micromagnetic Problems Using Projection-Based Finite Elements and Optimization on Manifolds

Müller, Alexander; Bischoff, Manfred; Keip, Marc-André 08:50
University of Stuttgart

We present a computational framework for the efficient numerical solution of the Landau-Lifshitz-Gilbert equation by exploiting projection-based finite elements [1, 2] and optimization on manifolds [3]. As a ample application, domain formation in cylindrical nanodots [4] is considered. The proposed framework leverages tools reported in our previous work on geometrically non-linear Reissner-Mindlin shells [5] and results in an efficient, robust and objective formulation.

The micromagnetic model is based on the vector potential and the magnetization director as independent fields. While the vector potential is embedded in the d-dimensional Euclidean space, the magnetization director resides on a d-1-dimensional manifold, that is, on the unit sphere embedded into the d-dimensional Euclidean space. The latter property comes along with a number of challenges associated with, for example, objectivity requirements and the geometrically meaningful integration in numerical schemes. Notably, the salient features of the magnetization prohibit the use of trigonometric functions for its spatial discretization.

In the present approach, we overcome the mentioned challenges by the use of projection-based finite elements and the optimization on manifolds, which specifically eliminates the need for explicit parameterization of the unit sphere. As a result, our formulation does not require any artificial constraints (often integrated by means of penalty formulations, renormalization strategies or Lagrange-multiplier methods [6, 7, 8]), but ensures a geometrically consistent representation of magnetization by the very definition of the search space. This definition, in turn, yields a further key advantage of our approach — the reduced number of degrees of freedom associated with the magnetization. In contrast to classical finite element implementations that require d degrees of freedom per node in d-dimensional space, our formulation copes with d-1 degrees of freedom per node. Taken altogether, our model facilitates computationally efficient yet accurate numerical simulations in micromagnetics and therewith offers promising avenues towards the realization of micromagnetic precision in large-scale practical applications. To showcase the efficacy of our formulation, we validate it with semi-analytical results of domain formation in cylindrical nanodots and apply it to a variety of more complex scenarios.

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Dual Weighted Residual Error Estimation for a Stationary Coupled Fluid Flow Heat System

Beuchler, Sven (1,2); Demircan, Ayhan (2,3); Endtmayer, Bernhard (1,2); Lankeit, Johannes (1); Wick, Thomas (1,2)

1: IfAM, Leibniz University Hannover
2: Cluster of Excellence PhoenixD, Leibniz University Hannover
3: Institute of Quantum Optics (IQO), Leibniz University Hannover

09:10

In this talk, we develop a posteriori error control for a nonlinear coupled fluid flow heat system in which density and viscosity are temperature-dependent. Therein, the stationary Navier-Stokes equations are coupled with a stationary heat equation. The coupled problem is modeled and solved in a monolithic fashion. The aim is to obtain goal oriented adaptivity and error estimates for one or possibly multiple goal functionals. The error localization is achieved with the help of a partition-of-unity in a weak formulation, which is specifically convenient for coupled problems as we have at hand. The error indicators are used to employ adaptive algorithms, which are substantiated with several numerical tests.

Thixoviscoplastic flow simulations based on Houska thixotropic and Bingham viscoplastic models

Begum, Naheed; Ouazzi, Abderrahim; Turek, Stefan

TU Dortmund University

09:30

In this talk, we discuss the solvability of thixoviscoplastic flow problems and provide FEM flow simulations.
Thixoviscoplastic flows based on Houska thixotropic and Bigham viscoplastic models are multifield nonlinear coupled problems. Beside the integrated nonlinearity within momentum and microstructure equations, thixoviscoplastic problems induce two way coupling. Such problems are often lacking unified FEM analysis due to the presence of different types of nonlinearities. Here, we analyze the solvability of auxiliary microstructure and viscoplastic subproblems with the corresponding suitable analysis tools which guarantee existence and uniqueness of solutions. Then, we proceed with the solvability of multifield coupled thixoviscoplastic problem. We provide TVP flow simulations in different configurations.

The material of this talk is based on our below recent work.

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Advanced PIV-based measurement method to determine fiber orientation in a transparent fresh concrete substitute liquid

Vaupel, Tim; Jacob, Simon; Gerland, Florian; Schomberg, Thomas; Wünsch, Olaf 09:50
University of Kassel

Today's ultra-high performance concretes are reinforced with fibers in order to build complex parts without reinforcement bars. The orientation of the fibers in the solidified concrete is essential for its resistance to certain forces.

Based on previous work by our working group [1,2], the fiber orientation in concretes and in substitute liquids was measured using different measurement methods. In addition, the influence of different fiber concentrations on the flow behaviour was investigated. It was found that fiber-fiber interactions occur more frequently at high fiber concentrations, resulting in an increase of the effective (unisotropic) viscosity.

In flow regions close to the wall at low shear rate, a deviation of the fiber orientation between numerical prediction and experimental observation was observed, requiring a more precise measurement methodology to improve the numerical modelling.

In order to study individual fibers and their orientation in detail in this field of research, a PIV-based measuring stand was built that is capable of analysing the orientation in a ball probe rheometer. A transparent substitute liquid containing tracer particles is used for this purpose. These particles can be used to capture the flow in a section plane using a camera and conventional methods of PIV measurement methods (cross correlation). At the same time, fibers are placed in the liquid. By refractive index matching the majority of the fibers, they disappear visually while at the same time, a small number of tracer fibers are added, which glow under the impact of UV light through phosphorescence. This makes it possible to observe individual fibers in the flow in detail and to record the interactions of the matrix liquid on the fibers and of fibers on the matrix liquid in detail.

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Port-Hamiltonian Modeling and Stability Analysis for Coupled Network PDAEs describing Gas Networks

Tischendorf, Caren; Pade, Jonas 10:10
Humboldt-Universität zu Berlin

We present a port-Hamiltonian modeling of gas networks in form of a partial differential algebraic equation system based on the mass flow balance equation and network element models describing the relation between enthalpy and mass flow. The set of network elements includes pipes, compressors, resistors and valves. We use the pipe model description from [1] that provides perturbation bounds via relative energy estimates.

Using the mixed-finite element spatial discretization part from the pipe discretization presented [2] we derive a port-Hamiltonian differential algebraic equation system. Finally, we present convergence criteria for a waveform relaxation approach for couplings of the resulting network DAEs exploiting the convergence result for coupled DAEs presented in [3, Theorem 2.4].

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S07.09.2: Coupling strategies

Date: March 22, 2024 08:30–10:30
Room: G22/H2
Chair(s): Radtke, Lars
Düster, Alexander

Convergence of waveform relaxation for coupled DAEs describing circuits with generalized elements

Pade, Jonas (1); Cortes Garcia, Idoia (2); Kumbhar, Pratik M. (3) 08:30
1: Humboldt-Universität zu Berlin
2: Eindhoven University of Technology
3: Vanderlande Industries Private Limited, India

Lumped circuit models are often used in electrical engineering to describe the behavior of certain devices. However, these models neglect spatially distributed electromagnetic phenomena, which, for some applications, is a too restrictive modeling assumption. In these cases, field/circuit coupling can be performed where fully spatially distributed electromagnetic field elements are coupled into a surrounding lumped circuit. Here, these field models can be understood as a type of generalization of classical circuit elements.
Cosimulation methods are well suited to solve field/circuit coupled systems since they allow for dedicated solvers and time scales for the different subsystems. A well-established family of iterative cosimulation methods is waveform relaxation. While waveform relaxation is convergent for coupled ordinary differential-equations on finite time intervals, it can diverge for coupled differential-algebraic equations unless an additional contractivity condition is satisfied. Computing the contractivity condition, however, is usually costly.
Here, we build on recent results concerning the classification of field models as so-called generalized circuit elements and circuit-topological convergence criteria for waveform relaxation on coupled circuits. Notably, we present an easy-to-check topological convergence criterion for coupled field/circuit systems, where the field can be classified as a generalized circuit element and the circuit is modeled by modified nodal analysis. If the convergence criterion is not satisfied, we have to expect waveform relaxation to diverge, or to converge comparatively slowly. For the case of slow convergence, accelerating strategies such as the optimized waveform relaxation method can be employed to speed-up simulation time. In addition to the topological convergence criterion, we present simulation results which confirm our theoretical findings for both convergent and divergent cases.

Towards model-based feedback control of hydrogels 3D bioprinting

Urrea-Quintero, Jorge-Humberto (1); Wick, Thomas (2); Wessels, Henning (1) 08:50
1: TU Braunschweig
2: Leibniz University Hannover

The emergence of 3D printing technologies has opened new frontiers in engineering functional materials for biomedical applications. Hydrogels, known for their biocompatibility, high water content, and adaptable mechanical properties, are at the forefront of this innovation. However, transitioning from laboratory prototypes to industrialized production poses significant challenges. These include maintaining consistent material properties across large-scale batches, optimizing print speeds, and ensuring reproducibility and uniformity in the final products.

We strive to advance the state of functional materials additive manufacturing by drawing on existing control-oriented modeling frameworks, model-order reduction techniques, the diffusion-deformation theory of soft materials, and feedback control theory for uncertain nonlinear systems. Consequently, we introduce a framework for model-informed 3D bioprinting, focusing on hydrogels. Our framework relies on a model that captures the coupled diffusion-deformation behavior of this

elastomeric material. Then, we create a reduced-order model using Proper Orthogonal Decomposition (POD), balancing computational efficiency with model fidelity, as preparation for the design of the feedback control algorithm.

In this contribution, we will discuss the numerical implementation of a coupled diffusion-deformation model and the construction of a reduced-order model. We use the FEniCS FEM package to solve the multiphysics model and RBniCS for the reduced-order model development.

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. We study the reduced-order model accuracy and analyze the speed-up in the simulation time compared to the high-fidelity model to determine its suitability for control applications.

We aim to bring complex mechanical models into the control loop, bridging the reproducibility and (real-time) quality control gap in bioprinting processes. Such integration is crucial for ensuring the final product adheres to the design specifications and possesses the necessary functional attributes. The ultimate goal is a closed-loop system that consistently yields high-quality, functional hydrogel products. The advancements in model-based bioprinting technologies are expected to enhance the reliability of bioprinting and make it viable for industrial-scale applications, such as fabricating human tissue analogs.

Macroscopic properties of solid oxide fuel cell electrodes via microstructure-based numerical homogenization

Langner, Eric (1); Makradi, Ahmed (2); Gouttebroze, Sylvain (3); Belouettar, Salim (2); Wallmersperger, Thomas (1)

1: TU Dresden
2: Luxembourg Institute of Science and Technology
3: SINTEF Industry, Norway

09:10

Due to climate change, a sustainable and energy-efficient energy supply is urgently required. Solid oxide fuel cells (SOFCs) - which are more efficient than other types of fuel cells - are promising energy converters that directly transform chemical energy into electrical energy. Experimental studies show that the characteristics of the microstructure of SOFC electrodes have a major impact on the macroscopic behaviour and are crucial for the overall performance of the fuel cell [1]. For this reason, we suggest which geometrical and physical properties needs to be determined in order to enable the incorporation of microscopic features into the macroscopic model. In particular, the composition and the respective volume fractions, the double/triple phase boundary as well as the tortuosity are important geometrical properties of the electrode [2]. The tortuosity is determined by the skeleton shortest path searching method. The effective physical parameters are determined by a first-order homogenization method. Important physical properties are the effective thermal, electric and ionic conductivities as well as the permeability for the gas. As these parameters are strongly dependent on the operating temperature, a multi-field first-order computational homogenization framework is developed and implemented in a finite element program. With these parameters, simulations can be performed at the fuel cell to find correlations between the microstructural characteristics (composition and morphology) and the performance.

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S08: Multiscales and homogenization

Organizer(s): Kaiser, Tobias *(TU Dortmund University)*
Schneider, Matti *(Universität Duisburg-Essen)*

S08.01: Material Modeling

Date: March 19, 2024 08:30–10:30
Room: G16/054
Chair(s): Scheunemann, Lisa

Numerical multiphase yield design modelling of reinforced soil structures: a focus on the interaction between soil and inclusions

Donval, Elodie (1); Hassen, Ghazi (2); de Buhan, Patrick (2) 08:30
1: University of Duisburg-Essen
2: Laboratoire Navier (Ecole des Ponts, UGE, CNRS), Marne-la-Vallée, France

Limit analysis (for elastic perfectly plastic materials) and yield design [1] (its extension to any kind of material) offer direct calculation methods and provide bounds to the extreme load of the structure. Their direct properties often lead to lower computational effort than other non-linear incremental methods. As such, they are convenient to use for engineers and are increasingly included in workflows for the design of geotechnical structures. Moreover, in some cases (reinforced concrete, masonry, reinforced soils for instance), the presence of reinforcements or joints makes the direct problem more difficult to mesh and solve. To mitigate this latter problem, one solution could be to resort to homogenisation. However, for inclusion-related problems, classical homogenisation has been shown to misestimate the overall strength of a reinforced structure because it does not account for debonding between the matrix and the reinforcing inclusions, nor for the bending strength of the inclusions. A way to take these features into account is to resort to a multiphase model [2], conceived as an extension of the periodic homogenization, in which the matrix and reinforcements are homogenized separetely as two interacting phases, modelled as a Cauchy and a Cosserat continuum respectively.

In this contribution, we present the numerical implementation of the multiphase model in the yield design framework and apply it to estimate the extreme load of a foundation subjected to a combination of a vertical loading, an horizontal loading and an overturning moment.

As a first step, the two phases and their mutual interaction strengths are estimated by solving a well-defined 3D auxiliary problem on a representative unit cell. Then, it becomes possible to evaluate the strength properties of a reinforced soil structure according to the multiphase approach, using a devoted f.e.m numerical code in which the static and kinematic approaches of yield design are implemented.

The so-developed numerical tool is used to determine the ultimate bearing strength of a piled foundation. Through such an example, it is possible to show how the interaction strength and the bending strength of the inclusions, which are directly related to their number, influence the extreme load of the whole structure.

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Comparative Analysis of Fracture Simulation Methods in Finite Element Models for Multiphase Materials and Multiscale applications

Najafi Koopas, Rasoul (1); Rezaei, Shahed (2); Rauter, Natalie (1); Ostwald, Richard (1); Lammering, Rolf (1) 08:50

1: Helmut Schmidt University, University of the Federal Armed Forces Hamburg
2: Access e.V.

This study investigates four fracture simulation methods applied to multiphase materials with interfaces within the finite element (FE) framework. The compared methods include the cohesive zone model (CZM) with zero-thickness cohesive interface elements, the standard phase field fracture model (SPFM), the cohesive phase field fracture model (CPFM), and a novel hybrid model that integrates CZM for interface debonding and CPFM for matrix cracking. The results show that CPFM is characterized by its effectiveness when the thickness of the interfacial zone is comparable to that of other phases. For materials with particularly thin interfaces, such as concrete on the meso or microscales, the hybrid model proves to be the most authentic numerical model. This investigation also shows that the CPFM method agrees well with the hybrid model in scenarios where the thickness of the interface is not excessively small. This indicates the potential of CPFM as a unified fracture approach for multiphase materials with homogenous phases. In addition, the study of the sensitivity of the integral load response of a representative volume element (RVE) with respect to the length-scale parameter shows that the CPFM integrates very well with multiscale frameworks, including those using convolutional neural network (CNN)-based homogenization techniques. This is emphasized by the advantages of CPFM in terms of lower computational cost compared to three other fracture methods and reduced implementation complexities when it is compared to CZM and hybrid approaches. This efficiency and simplicity make CPFM an attractive choice for complex multiscale modeling applications.

Analytical strain localization for inhomogenous eigenstrains in lamellar materials

Klein, Claudius; Dyck, Alexander; Böhlke, Thomas 09:10

Karlsruhe Institute of Technology

Towards the goal of quantitative prediction of macroscopic mechanical properties, efficient simulation models are necessary, which take the influence of the materials microstructure into account [1]. In this talk we focus on metallic materials with lamellar structures, such as NiAl-Cr(Mo) or binary Fe-Al alloys. These consist of individual grains, which are arrangements of periodic layers with a distinct layer normal direction. The interfaces between the layers act as obstacles for dislocations, which, in combination with the small layer thickness (micrometer range), lead to a dislocation pileup and therefore to an inhomogeneous distribution of the plastic deformation within each layer.

The accurate prediction of strain localization is of interest as it enables taking pileup effects into account in material models. We present an analytical homogenization scheme, which takes both the material contrast of the individual phases and the local inhomogeneous plastic strain distribution into account. This allows the determination of the local stress and strain fields on the microscale which are generally inhomogeneous in the layers and discontinuous at the interfaces. We make use of the established laminate theory to describe a single grain as a rank-1 laminate instead of spatially resolving the individual layers, allowing for an efficient description of the mechanical behavior. The scheme extends the approach for an elastic laminate from Glüge and Kalisch [2] by inhomogeneous plastic strains and makes use of the interfacial operators introduced by Hill [3]. We derive explicit expressions for the local stress and strain fields, allowing for detailed insight into the complex deformation behaviour of a single grain with heterogeneous fields.

Lastly we compare the analytical solution with full field finite element simulations of lamellar structures with a prescribed distribution of the plastic deformation and discuss the results.

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Numerical polyconvexification of isotropic damage

Balzani, Daniel (1); Köhler, Maximilian (1); Neumeier, Timo (2); Peter, Malte A. (2); Peterseim, Daniel (2); Wiedemann, David (3)

1: Ruhr University Bochum
2: University of Augsburg
3: TU Dortmund University

09:30

Finite element simulations of pseudo-time-incremental damage models in the finite strain setting often suffer from mesh dependence and stability issues caused by the non-convexity of the underlying energy densities. This talk will focus on the relaxation of such a model and discuss algorithms that are used to approximate semi-convex hulls, like the polyconvex envelope. The computational complexity of (semi-)convexification algorithms is substantially affected by the computational dimension. Operating within the d x d dimensional space of the deformation gradient makes it unfeasible to perform a large finite element simulation at this stage due to the computational resources required.

We present a feasible method to determine the polyconvex envelope in the presence of isotropy. The method is based on the characterisation of the energy density in terms of signed singular values. The practical algorithm requires only the computation of the lower convex envelope of a d-dimensional manifold. This convexification can be realised by computational geometry algorithms or an optimisation approach. Reducing the dimensionality from d x d (matrix space) to d (signed singular value space), computation is significantly accelerated and this speedup makes the complete simulation of boundary value problems feasible. First findings on the application to the isotropic damage model, regarding the mesh sensitivity of the numerical approximations, will be presented.

Morphology-Based Homogenization of Thermodynamic Driving Forces and Mechanical Properties in Phase Transforming Materials

von Oertzen, Vincent; Kiefer, Bjoern

TU Bergakademie Freiberg

09:50

The macroscopic behavior of phase transforming solids strictly depends on characteristic microscopic evolution processes—such as twinning, reorientation, solidification or decomposition phenomena—during which the microstructure topology changes over time. The thermodynamic properties of these multi-physical mechanisms have been extensively studied over the last decades for a variety of multifunctional material systems, see [1,2] and the references therein. The majority of existing models relies on transient and spatially-regularized phase-field approaches, so that large-scale simulations are usually associated with enormous computational costs, since the involved temporal and spatial scales need to be resolved numerically with sufficient accuracy. Consequently, the embedding of existing routines into modern two-scale approaches, such as the FE^2-method, is immensely constrained by technical limitations. Moreover, a general notion for consistently transferring specific phase-field models between multiple, variable scales has still not been fully developed.
To overcome these issues, the recently introduced concept of unequally and nonlinearly weighted averaging operators [3] provides a promising homogenization framework. Here, this rather general approach is used to derive macroscopic relations for the displacive dual-phase system ZrO_2. More specifically, it is mathematically demonstrated that macroscopic driving forces as well as effective mechanical properties can be expressed as functions of the average martensite volume fraction and, additionally, of a finite collection of weighted phase averages—so-called phase-morphologies. In this regard, the structure and number of the corresponding weighting functions, necessary to obtain such unique macroscopic relations vary based on the complexity of the microscopic phase distributions. The validity of these theoretical results is demonstrated through finite element simulations of microstructure formation in the given material system. These numerical simulations are performed for various temperature- and strain-controlled loading scenarios.

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Rate-dependent effects in micromechanical constitutive multiscale modeling of ferroelectrics

Warkentin, Andreas; Ricoeur, Andreas
University of Kassel

10:10

Ferroelectrics exhibit many interesting effects, both linear and nonlinear, which is why these materials are widely used in science and industry. Moreover, it is noteworthy that the majority of these effects, particularly those which are nonlinear, are strongly rate-dependent, rendering the modeling of these intricate materials with multiple material scales quite challenging. The rate dependence is contingent on the material scale at which these distinct effects occur, yet they are all reflected in the macroscopic material behavior. Furthermore, nonlinear effects are irreversible and are accompanied by energy dissipation, which generally leads to a temperature rise of the material. For modeling the distinctive nonlinear rate-dependent effects of ferroelectric materials, there are numerous options, including microphysical and phenomenological models.

Aspects of different rate-dependent effects, as well as mutually coupled dissipative processes in ferroelectrics, in particular ferroelectric domain switching and viscoelasticity, are investigated theoretically, based on a microphysical motivated thermo-electromechanical multiscale constitutive framework.

For this purpose a hybrid micromechanical–rheological constitutive model is developed and embedded in the framework of a multiscale modeling approach [1, 2, 3]. The mathematical theory is consistent against the background of rational thermodynamics and deals with two types of internal variables. The advanced modeling approach is inter alia applied to identify novel energy harvesting cycles exploiting dissipative effects, resulting in a major electric work output.

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S08.02: Microstructure

Date: March 19, 2024 16:30–18:30
Room: G16/054
Chair(s): Waimann, Johanna

Microstructure reconstruction for realistic RVEs: harnessing descriptor differentiability

Seibert, Paul; Raßloff, Alexander; Kalina, Karl; Kästner, Markus
TU Dresden

16:30

Microstructure reconstruction and characterization (MCR) provides realistic microstructure realizations for multiscale simulation and accelerating materials engineering. Common use-cases are (i) creating a 3D computational domain from 2D data such as a microscopy image; (ii) reconstructing a small, periodic domain from a large, aperiodic CT scan; (iii) creating a set of statistical volume elements from a single reference; and (iv) enhancing microstructure datasets by sampling and interpolating in the descriptor space. Descriptor-based MCR is a subclass of methods that aims at accomplishing all of these four goals. The main advantage over machine learning-based MCR is that no data set is needed. Instead, it can be used to create it, making data-driven modeling and simulation possible on otherwise insufficient amounts of data.

After a brief introduction to the underlying concepts, the potential of differentiable descriptors is analyzed in depth. Naturally, it makes the use of gradient-based optimization algorithms possible, reducing the number of iterations by orders of magnitude when compared to the Yeong-Torquato algorithm [1,2]. This is discussed alongside with a validation [3] and an implementation [4]. However, this requires solving a new optimization problem for each realization of a material structure. As an alternative, a method is proposed where a neural cellular automaton is trained to identify a PDE system that generates structures very efficiently. Therein, the descriptors define the loss function and not data set us required. Finally, rethinking the problem definition, a sequential gradient projection based method from the texture synthesis literature is identified as a viable microstructure reconstruction algorithm and an extension from 2D to 3D is developed. This increases the computational and memory efficiency even further.

[1] Seibert et al., Reconstructing random heterogeneous media through differentiable optimization, COMMAT, 2021

[2] Seibert et al., Descriptor-based reconstruction of three-dimensional microstructures through gradient-based optimization, Acta Materialia, 2022

[3] Seibert et al., Two-stage 2D-to-3D reconstruction of realistic microstructures: Implementation and numerical validation by effective properties, CMAME, 2023

[4] Seibert et al., Microstructure Characterization and Reconstruction in Python: MCRpy, IMMJ, 2022

[5] Seibert et al., Fast reconstruction of microstructures with ellipsoidal inclusions using analytical descriptors, CADJ, 2023

Active learning for inverse mesostructure design

Raßloff, Alexander; Seibert, Paul; Kalina, Karl; Kästner, Markus
TU Dresden

16:50

In this contribution, we propose a general framework to inversely designing structures using structure-property linkages. For deriving profound correlations, large databases are necessary. Experiments alone are prohibitively expensive. Therefore, computational augmentation is employed to allow for data-driven approaches even in this data scarce regime.

In an iterative approach (1) mesostructures are characterized by descriptors, (2) effective properties are derived from numerical simulations, (3) structure-property linkages are set up using a Gaussian process, (4) descriptors ofnew candidates mesostructures are proposed by Bayesian optimization and (5) mesostructures are reconstructed. Steps 2 through 5 are repeated until a desired convergence criterion is reached, e.g., the uncertainty of the structure-property linkage is decreased or a mesostructured with preferable properties is found.

This framework is applied and presented at the example of spinodoid structures. Augmenting a small initial data set by in silico reconstructed microstructures and their simulated effective properties allows for deriving improved structure-property linkages and, thus, finding potentially optimal microstructures or predicting properties.

Fiber orientation-length coupling in short-fiber reinforced composites

Mehta, Alok Ranjit; Schneider, Matti
University of Duisburg-Essen

17:10

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. Injection molding process is used widely to produce intricate parts with such materials. The process inherently generates complex microstructure which might have layered constituents (skin-core-skin), different fiber-lengths due to fiber breakage during the injection process and different fiber-orientations due to flow of the matrix material. It is evident from the µCT images that in SFRP, shorter fibers orient more or less randomly whereas longer fibers orients strongly in the direction of

the flow [5]. 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 [4] can be used to generate digital image of the microstructure which is then used in conjunction with FFT based coputational homogenization methods to compute effective material properties. An extension of the SAM Algorithm which originally assumes uncoupled behavior [2] for fiber-length and fiber-orientation distributions is studied and presented. In this work coupled behavior is discussed using different fiber-length distributions. Also effects on mechanical properties for coupled and uncoupled approaches are compared and analyzed. Results are validated by experimental evaluations done by Hessman et al. [1] and M¨uller[3].

References:

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Microstructure generation for discontinuous long curved fiber-reinforced polymers via optimization on curved manifolds along the geodesics

Lauff, Celine (1); Schneider, Matti (2); Böhlke, Thomas (1) 17:30

1: Karlsruhe Institute of Technology
2: University of Duisburg-Essen

Discontinuous long fiber-reinforced composites are frequently used for lightweight applications due to the high specific stiffness to weight ratio and the cost-efficient manufacturing processes [1]. Using micro-CT imaging to characterize their microstructure shows that the material is highly anisotropic, heterogeneous and random on the microscale. To determine the anisotropic mechanical properties of such heterogeneous materials, computational multiscale methods are indispensible tools. However, a complete geometrical description of the microstructure is necessary first.

Such a geometrical description may be obtained via microstructure generation, complementing data from micro-CT imaging. Based on an optimization scheme, the Sequential Addition and Migration (SAM) algorithm for long curved fibers [2] offers a representative realization of the desired descriptors, i.e., the fiber volume fraction and the length and orientation distributions. To account for the fiber curvature, the fibers are discretized as polygonal chains, where the segments move separately during the optimization. To enforce the coherence between adjacent segments for convergence, an additional penalty term is added to the objective function. However, this disconnected fiber motion leads to convergence problems. Thus, for industrial aspect ratios and fiber orientation distributions, the necessary fiber volume fractions are barely achievable.

To enable microstructure generation for long fiber-reinforced composites used in industry, we present an innovative approach requiring that the coherence condition is fulfilled in every iterative step. Thus, the motion is restricted to a curved manifold. For such an optimization problem, the classical gradient descent iterates may leave the optimization space. To compute admissible iterates, we adapt the gradient descent scheme for a motion along the geodesics, i.e., the shortest lines between two points on the manifold. Therefore, we first derive the equations governing the geodesics in

form of d'Alembert type constrained mechanical systems [3]. Then, we discuss the efficient numerical treatment and the integration of the novel strategy into the SAM algorithm.

References:
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Quantification of Microstructure-Related Uncertainties in Macroscopic, Structural Quantities of Interest based on Artificial Microstructures and the FE2-Method

Dorn, Hendrik; Miska, Niklas; Balzani, Daniel 17:50
Ruhr University Bochum

Variability of microstructure morphology, which is inherently associated with the production process, leads to an uncertain mechanical response locally varying over the macroscopic structure. Such uncertainties have a strong influence on macroscopic quantities of interest, which are e.g., to be computed in terms of comparative measures to analyze failure of structural components. To quantify this influence, in this contribution, we propose to apply a method [3] for the construction of a set of artificial microstructures matching the real material's microstructure variation and use this set in the context of FE2 to represent macroscopic random fields. The set is obtained by generating statistically similar volume elements similar to the approach in [1] until the distribution of statistical variation in terms of statistical microstructure descriptors of higher order reflects the real material's distribution. The main benefit of chosing artificial microstructures over real microstructures as RVEs is the reduced morphological complexity and thus, improved numerical efficiency. In order to avoid the manual construction of suitable, conforming meshes for each of these microstructures, the Finite Cell Method is applied on the microscale. To reduce the number of subcells, an optimal decomposition algorithm is considered to determine a minimal set of subcells from microstructural voxel data, cf. [2]. To quantify the uncertainties at macro-structural level, various macroscopic random field realizations in terms of sets of artificial RVEs considered in the concurrent microscopic finite element problems are evaluated. The method is demonstrated for a sheet metal forming problem of a DP steel.

[1] D. Balzani, L. Scheunemann, D. Brands, and J. Schröder. Construction of two- and three-dimensional statistically similar RVEs for coupled micro-macro simulations. Computational Mechanics, 54(5):1269–1284, 2014.

[2] Y. F. Fangye, N. Miska and D. Balzani. Automated simulation of voxel-based microstructures based on enhanced finite cell approach. Archive of applied mechanics, 90:2255-2273, 2020.

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Aspects of numerical efficiency and viability in the optimization of minimal-surface-based periodic microstructures

Krischok, Andreas; Yaraguntappa, Basavesh; Keip, Marc-André 18:10
University of Stuttgart

Inspired by lattice structures that are observable in nature, micro-porous materials have been causing an ever increasing interest in the recent years. This is not least due to the fact that the production of such materials becomes more and more feasible by means of additive manufacturing. In this regard, 3D-printed structures with graded volume fractions have been shown to provide superior properties

in the context of providing an optimal compliance if subjected to non-homogeneous deformations but are likely to be inferior to optimized solids without a cell structure.

Since the optimal configuration of microscopic unit cells under heterogeneous macroscopic stress states will be nonlocal and anisotropic, one needs to design microstructures in a locally adaptive manner. We tackle this problem by means of a phase-field approach for the optimization of microstructures based on triply-periodic minimal surfaces. In that regard, it is out goal to obtain unit cells with a locally optimal homogenized stiffness with respect to the direction of the maximum principal stress. In the present contribution, we will show that different kinds of optimized microstructures exhibit fundamental differences with regard to their response to tension- or shear-dominated loads. In this context, we discuss ways to identify viable solutions that prevent failure mechanisms due to disconnected cells. Furthermore, we will discuss strategies to verify the gain of the stiffness response experimentally.

S08.03: Model Order Reduction

Date: March 20, 2024 08:30–09:30
Room: G16/054
Chair(s): Hellebrand, Sonja

Statistically compatible hyper-reduction for computational homogenization

Wulfinghoff, Stephan 08:30
Kiel University

The computational bottleneck of reduced order models (ROMs) in nonlinear homogenization is usually given by the local material laws, which need to be evaluated in a large number of microscopic integration points. Hyper-reduction methods use only a small subset of the integration points and reach tremendous speed-ups at high accuracy. However, the underintegration breaks the overall compatibility of the microscopic strain field and is in this sense disrespecting the microscopic boundary value problem. Here, a new type of generalized integration points is introduced in strain space in order to remedy this shortcoming. Being inspired by results from nonlinear homogenization theory, the concept of *statistical compatibility* is developed and forms the theoretical basis for the new integration points, which respect the compatibility of the microscopic strain field in a statistical sense. The statistically compatible integration points can be derived offline and replace the conventional ones in a Galerkin-projection based setting with global modes identified via proper orthogonal decomposition (POD). The method is tested for various reinforced composites, indicating that 10-20 integration points are often sufficient to reach errors smaller than 3%, with CPU-times in the μs-range (per time step). A possible extension of the method for problems with higher nonlinearity and stronger field fluctuations is discussed within the context of a porous microstructure.

Nonlinear model order reduction using manifold learning techniques for computations on representative volume elements

Faust, Erik; Scheunemann, Lisa 08:50
RPTU Kaiserslautern-Landau

Manifold learning techniques which can extract nonlinear information from high-dimensional data – such as Laplacian Eigenmaps (LEM) and Locally Linear Embedding (LLE) – are popular in image and speech processing [1]. Recently, these methods have also been successfully exploited for projection-based model order reduction in fluid mechanics [2] and elastodynamics [3].

In the context of computations on representative volume elements (RVEs) for computational homogenisation, LEM and LLE can capture nonlinearities in solution manifolds using a lower-dimensional parametrisation than established linear techniques such as the proper orthogonal decomposition (POD). Their robustness in cases with comparatively little training data is especially interesting. Competing methods utilising neural networks [4] require comparatively large amounts of data, and the clustering step required for the generally very successful local basis methods [5] may

also be sensitive in data-poor applications. As a result, manifold learning techniques may be particularly well-suited to the construction of physics-based surrogates using which faster, lower-fidelity models can be trained.

In this contribution, we explore the application of LEM and LLE to representative volume element computations. Nonlinear behaviour, including hyperelasticity and elastoplasticity, is considered. The performance of the manifold learning techniques as well as the POD and local basis methods are compared for simple RVE examples.

[1] Lee, John A., and Michel Verleysen. Nonlinear dimensionality reduction. Vol. 1. New York: Springer, 2007.

[2] Pyta, Lorenz Matthias. "Modellreduktion und optimale Regelung nichtlinearer Stro̊mungsprozesse." PhD diss., Dissertation, RWTH Aachen University, 2018.

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A Comparative Study Between a Phenomenological, a Hybrid Neural Network and a Hyper ROM FE² Approach for Multiscale Simulations

Lange, Nils (1); Hütter, Geralf (1,2); Abendroth, Martin (1); Malik, Alexander (1); Kiefer, Bjoern (1) 09:10
1: TU Bergakademie Freiberg
2: BTU Cottbus-Senftenberg

Numerical homogenization represents a common way of capturing the mechanical response of a structure with a distinct scale separation, by localizing the state on the higher scale, solving the boundary value problem at the lower scale and transferring the result back. While the FE² method possesses a high degree of generality, the great computational effort limits its use in many practical applications, so that approximation techniques often have to be employed.

Finding methods, which accurately reproduce the FE² solution also in highly irreversible processes and keep its intrinsic flexibility, while requiring much less computational resources, is a challenging task. Machine Learning based approximation methods that incorporate certain physical information, such as Reduced-Order Models (ROM) or Physics-Informed Neural Networks (PINN), are promising alternatives. Although all approximation methods rely on a certain amount of full FEM solutions in an offline stage as training data, the amount of required data, flexibility of the particular models, their predictive and extrapolation capabilities and computational costs are quite different.

Multiple approaches are compared in the present study with respect to those criteria, among them a phenomenological model with material parameters fitted to training data [1], a hybrid neural network model [2], and a hyper-integrated reduced-order modeling FE² scheme [3]. The individual advantages and disadvantages of the methods are illustrated by means of representative 3D numerical examples modeling different material types.

[1] Abendroth, M., Malik, A., Kiefer, B., *A Modified Ehlers Model for the Description of Inelastic Behavior of Porous Structures*, arXiv, doi:10.48550/arXiv.2307.10216, 2023.

[2] Malik, A., Abendroth, M., Hütter, G., Kiefer, B., *A Hybrid Approach Employing Neural Networks to Simulate the Elasto-Plastic Deformation Behavior of 3D-Foam Structures*, Adv. Eng. Mat., doi:10.1002/adem.202100641, 2021.

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S08.04: Machine Learning

Date: March 20, 2024 14:00–16:00
Room: G16/054
Chair(s): Ostwald, Richard

Machine learning for the forward and inverse homogenization of cellular materials

Kochmann, Dennis M. (1); Zheng, Li (1); Bastek, Jan-Hendrik (1); Kumar, Siddhant (2) 14:00
1: ETH Zurich
2: TU Delft

Predicting the effective, homogenized mechanical properties of cellular structures and archtiected materials as well as identifying specific structural designs that meet target properties are common challenges in solid and structural mechanics. We will discuss the application of machine learning (ML) to those challenges and present opportunities for bypassing expensive computational modeling through the use of ML-based models. Specifically, we will present the use of Variational Autoencoders combined with a graph representation of trusses to predict and optimize the homogenized anisotropic stiffness and the homogenized nonlinear stress-strain response of general periodic truss lattices. The introduction of a low-dimensional and interpretable latent space representation of periodic trusses allows us to not only perform efficient property optimization but also to interpolate between dissimilar designs. In addition, we will show how video diffusion models can predict optimal cellular structures with as-designed homogenized nonlinear stress-strain response. In this case, the ML-based model not only efficiently identifies optimal designs with target properties but also predicts the full-field stress and strain distribution inside the sample, thus bypassing the optimization step as well as the full-field finite element simulation. In both cases, we demonstrate that the generative ML models generalize well outside the training set, meaning that new designs can be predicted with properties not encountered during training the neural networks.

From microgeometry to macroscopic modeling of porous materials enhanced by deep neural networks

Heider, Yousef; Aldakheel, Fadi 14:40
Leibniz University Hannover

Within the multiscale simulation of multiphase porous media, the underlying work focuses on Artificial Neural Network (ANN) applications to generate material models or predict macroscopic characteristics via supervised machine learning (ML). While feed-forward regression neural networks (FFNN) can be applied for capturing the history-independent material parameters, such as the permeability tensor, the recurrent neural networks (RNN) or the 1D Convolutional Neural Networks (CNN) can be used to capture history-dependent responses, such as the retention model [1,2].

The database used in the current supervised machine learning (ML) relies on the lower scale one- and two-phase lattice Boltzmann (LB) simulations, applied to deformable and anisotropic representative volume elements (RVEs) of the porous materials (Bentheimer networks). A special focus in this is on the anisotropy and deformation dependency of the intrinsic permeability tensor.

Alternative to the feed-forward regression model that relied entirely on the LB outputs, we will utilize in this work two-dimensional Convolutional Neural Networks (CNN) to predict the macroscopic anisotropic permeability tensor at different deformation states. In analogy to [3,4], the inputs for the CNN model consist of binarized CT images of real microgeometry, whereas the output is the symmetric 2nd-order permeability tensor. Thus, the presentation will discuss the capability of the ML model to generate a universal permeability model that relies on a limited number of CT images of the real microgeometry to capture the Darcy and non-Darcy flow in deformable and anisotropic porous materials.

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[4] Aldakheel, F., Elsayed, E.S., Zohdi, T.I. et al. (2023): Efficient multiscale modeling of heterogeneous materials using deep neural networks. Comput Mech 72, 155–171.

A Machine Learning Approach for a Statistical Homogenization Method for Elastic Two-phase Materials

Schmollack, Luzie; Klinge, Sandra 15:00
TU Berlin

Statistical homogenization methods are widely used to predict the response of a heterogeneous material to loading. To apply the methods, a key challenge is the choice of the right correlation function. Limitations in experimental and theoretical tools often lead to difficulties in finding a good approximation of the statistical descriptor.
We propose an approach that employs machine learning techniques to address the difficulty of finding the correct statistical descriptor for a class of 2D two-phase-microstructures. A neural network is used to extract the probability functions from the microstructure image.

Multiscale modeling of anisotropic finite strain elasticity with physics-augmented neural networks and generalized structure tensors

Kalina, Karl (1); Brummund, Jörg (1); Sun, WaiChing (2); Kästner, Markus (1) 15:20
1: TU Dresden
2: Columbia University, USA

The formulation and calibration of constitutive models is still a challenging task for materials which exhibit complex nonlinear behavior. Due to this, numerous novel approaches, generally referred to as data-based or data-driven methods, have been developed in the computational mechanics community recently. Thereby, a promising field of application is the usage of such methods for the acceleration of multiscale simulations [1]. Herein, we present an approach based on physics-augmented artificial neural networks (ANNs) as macroscopic surrogate models [2].

Our approach allows the efficient simulation of materials with complex underlying microstructures which reveal an overall anisotropic and nonlinear behavior on the macroscale. Thereby, we restrict ourselves to finite strain hyperelasticity problems here. By using a set of problem-specific invariants as the input of the ANN and the Helmholtz free energy density as the output, several physical principles, e.g., objectivity, material symmetry or thermodynamic consistency are fulfilled a priori [1,2]. The invariants are formed from generalized structure tensors and the right Cauchy Green deformation tensor. Necessary data for the training of the ANN-based surrogate model, i.e., macroscopic deformations and corresponding stresses, are collected via computational homogenization of representative volume elements (RVEs). Besides the network parameters, the structure tensors are automatically calibrated during training so that the underlying anisotropy of the RVE is reproduced in the best possible way. The developed approach is exemplarily applied to several descriptive examples.

[1] Kalina, K. A., Linden, L., Brummund, J., Kästner, M.: Computational Mechanics 71 (2023), https://doi.org/10.1007/s00466-022-02260-0.

[2] Linden, L., Klein, D. K., Kalina, K. A., Brummund, J., Weeger, O., Kästner, M.: Journal of the Mechanics and Physics of Solids 179 (2023), https://doi.org/10.1016/j.jmps.2023.105363.

Surrogate elements for nonlinear microstructures using physics-enhanced machine learning

Li, Wei; Weeger, Oliver
TU Darmstadt
15:40

For microstructured materials with non-periodic cells or non-separated scales, such as additively manufactured lattices and metamaterials, multiscale modeling approaches are inapplicable, but full-scale simulations are still prohibitively time-consuming, in particular for nonlinear materials and large deformations. For a fast and efficient nonlinear simulation of such structures, similar to [1], we introduce the concept of surrogate elements, which capture the effective mechanical behavior of the unit cells of the microstructure only through the boundary nodes. We consider an internal energy potential, which enables the determination of the energy and (generalized) forces associated with a given deformation of the microstructure's boundary nodes. This potential is represented by feed-forward neural network (FFNN) that incorporates energy conservation, invariance to rigid body translations and rotations, normalization conditions, and parameter variations of the unit cells, i.e., through physics-enhanced machine learning. The equilibrium configuration of a macro-structure consisting of many interconnected unit cells can then be obtained by minimizing the total potential energy, which is assembled from the microstructure potentials.

Here, this concept is demonstrated in application to 2D and 3D beam lattice microstructures. First, a data set for the surrogate potential, forces, and moments is build by performing nonlinear simulations of lattice unit cells subject to different deformation and load cases. Then, a physics-enhanced neural network is trained on this data in order to approximate the functional relationship for the energy potential. We aim to demonstrate the accuracy, efficiency and robustness of the approach through several verification examples, in which these surrogate potentials are applied for the nonlinear simulation of macro-structures.

[1] G. Capuano and J. J. Rimoli. "Smart Finite Elements: A Novel Machine Learning Application". Computer Methods in Applied Mechanics and Engineering 345:363–381 (2019)

S08.05: Interfaces/Size Effects/Higher-Order Continua

Date: March 20, 2024 16:30–18:30
Room: G16/054
Chair(s): Meyer, Knut Andreas

Revisiting Cohesive composite boxels with imperfect interfaces: Challenges and Limitations

Keshav, Sanath (1); Fritzen, Felix (1); Kabel, Matthias (2)
1: University of Stuttgart
2: Fraunhofer ITWM
16:30

The realm of FFT-based simulations for modeling interfacial damage has long been challenged by the need for accurate and efficient methodologies. Bridging this gap, a novel framework integrating cohesive zones with composite boxels [Keshav, S. Fritzen, F. Kabel, M. 2022] and an innovative image-based algorithm was developed, aiming to surpass the constraints of cartesian discretization prevalent in FFT methods. This approach along with similar works [Chen, Y. Gélébart, L. Marano, A. Marrow, J. 2021] initially promised a significant advancement in aligning the precision of classical cohesive elements with the demands of finite element simulations. However, a deeper dive into this methodology has revealed a series of substantial theoretical and practical challenges, casting new light on its efficacy and applicability. This presentation is set to explore these revelations, delving into the nuances and intricacies of cohesive zone models within FFT-based solvers.

Influence of grain boundaries on the overall diffusivity in polycrystalline solids

Scholz, Lena; Ou, Yongliang; Grabowski, Blazej; Fritzen, Felix 16:50
University of Stuttgart

Major progress in battery technology is a key to the decarbnoization 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 multiphyiscal multiscale effects within the solid-state electrolyte is subject of research across various disciplines.

The diffusion behavior of Li ions in the solid-state electrolyte is crucial for the overall performance of the battery. In rthe literature the details of the polycrystalline structure on larger scales are often neglected or only considered under strong assumptions such as isotropy. However, the results of studies on smaller scale, such as the one by Dawson and Islam [1], indicate that grain boundary effects and, therefore, the grain size do have a significant impact on the overall diffusivity. Despite its promising insights, the atomistic simulations used in the mentioned study go along with massive computational demands, thereby limiting the size of the studied cells considerably.

Our approach considers the fully resolved crystalline structure to find a microscopic description that accounts for diffusion along as well as across grain boundaries. This is embedded into a finite element simulation by introducing a novel interface element. The results are governed by different and potentially anisotropic diffusion coefficients in bulk and grain boundary domains gained from ab initio calculations. 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. An in-depth analysis on the material and structural features that govern the effective diffusion behavior in this model enables the application of data-integrated techniques and the design of meaningful surrogate models. Hence, the concepts on the different scales as well as computational and experimental results are brought closer together. 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. 2424-231, 2022

A computational homogenisation approach accounting for interfaces in electrical conductors

Güzel, Dilek (1); Kaiser, Tobias (1); Menzel, Andreas (1,2) 17:10
1: TU Dortmund University
2: Lund University

Every material in nature exhibits heterogeneous behaviour at some scale. The effective material response is governed by the underlying microstructure. Interfaces, such as phase and grain boundaries, can affect the overall response of the material under consideration. Grain boundaries are particular sources of resistance in polycrystalline materials with empirical evidence suggesting that grain boundaries can substantially influence the electrical properties [1,2]. Computational multiscale formulations allow complex microscale processes and distinct features such as material interfaces at the microscale to be accurately resolved in simulations.
Motivated by the influence of grain boundaries on effective electrical properties, a computational multiscale framework for electrical conductors is extended to continua with material interfaces at the microscale [3]. In particular, (lowly-conducting) cohesive-type interfaces are accounted for at the microscale, such that displacement and electrical potential jumps across the interface can be considered. The thermodynamic fundamentals of continua featuring cohesive-type interfaces in a small deformation setting are provided. Based on these, a computational multiscale framework is established. Specifically speaking, averaging theorems for the mechanical and electric field quantities are derived and consistency with the Hill-Mandel condition for suitable boundary conditions is discussed.

By means of scale-bridging relations, the macroscopic quantities are expressed as surface integrals. It is demonstrated that the boundary integrals remain identical to their form in first-order homogenization.
To demonstrate the capabilities of the proposed framework, various representative boundary value problems are examined. In particular, a study on characteristic size effects is presented and the simulation results are validated by means of a quasi one-dimensional analytical solution. To investigate deformation-induced property changes at the microscale, a typical [1-d]-type damage formulation is assumed for the electrical conductivity at the interface. This eventually enforces the coupling between the electrical and mechanical subproblem at the material interface.

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Single-species diffusion in particle-matrix composites using a dual-potential model from computational homogenization

Rollin, David (1); Larsson, Fredrik (2); Runesson, Kenneth (2); Ekre, Fredrik (1); Jänicke, Ralf (1) 17:30
1: TU Braunschweig
2: Chalmers University of Technology, Sweden

There is a variety of applications for complex diffusion problems in particle-matrix composite materials, for example, ion transport in a porous battery electrode. Directly simulating such processes for a problem on the application scale with full microstructural resolution is often computationally not feasable. One approach to reduce the cost is computational homogenization.

There are different approaches to describing diffusion in composite materials. In this study, we investigate linear diffusion processes driven by a chemical potential. We consider processes at the particle-matrix interface, such as chemical reactions, that give rise to a jump in chemical potential at the interface.
The two-scale framework is derived by applying the concept of variationally consistent homogenization. On the sub-scale we consider a Representative Volume Element (RVE) and assume microstationarity. In this case, transient effects due to the flux through the interface are captured by an effective source term in the large-scale equations. Due to the model's linearity, the effective response of the RVE can be computed by direct upscaling via sensitivities. On the large scale, we use a formulation with two chemical potentials for the different materials to account for the possible jump in chemical potential at the particle-matrix interface.

In this case, we apply first order homogenization for both large-scale potentials. However, the discontinuity of the particle phase gives reason to investigate different formulations of the homogenization for this phase. We investigate three different approaches: standard first order homogenization, a variation which prescribes the large-scale potential gradient as moment of the potential, and a constant prolongation of the large-scale potential.

First, we investigate the response of a two-dimensional RVE for the different approaches to demonstrate the difference in behavior. Then, we compare the large-scale models with the results of a direct numerical simulation for an example problem. Since the overall behavior depends on the ratio of material parameters, this is done for multiple parameter sets.

Investigation of elastic and inelastic size effects in composites using micromorphic multi-scale simulations

Malik, Alexander (1); Hütter, Geralf (1,2); Abendroth, Martin (1); Kiefer, Bjoern (1) 17:50
1: TU Bergakademie Freiberg
2: BTU Cottbus-Senftenberg

The properties of two-phase materials, with the special case of foams, strongly depend on their microstructure and are known to exhibit size effects. In general, these structures are modeled with Hill homogenization methods to reduce the computational effort compared to full-resolution (high-fidelity) simulations. For applications where the macroscopic dimensions of the structure under consideration are only a few multiples of its internal length, such size effects must be taken into account, since the effective mechanical properties then depend on the internal structure size. In order to achieve adequate homogenization, higher-order continuum theories can then be used to account for strong gradients in mechanical quantities. The present contribution builds on a Direct FE^2 implementation [1] to extend the classical approach with the corresponding micromorphic degrees of freedom while relying on the functional scope of the utilized software. Elastic-plastic material behavior is investigated with Cosserat and an unrestricted micromorphic theory [2,3]. Simple loading cases, such as pure bending, are investigated and compared with partly existing analytical solutions. More complex examples in the large deformation setting are examined in order to determine the theory's limits of validity. Direct numerical simulations of the corresponding fully-resolved structure are considered as a reference.

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S08.06: Machine Learning/TFA/Mean-Field

Date: March 21, 2024 08:30–10:30
Room: G16/054
Chair(s): Wulfinghoff, Stephan

Thermo-mechanically coupled Nonuniform Transformation Field Analysis of heterogeneous solids

Fritzen, Felix (1); Herb, Julius (1); Sharba, Shadi (2) 08:30
1: University of Stuttgart
2: Fraunhofer ISC

The Nonuniform Transformation Field Analysis (NTFA) was first presented two decades ago. It extends Dvorak's Transformation Field Analysis by accounting for a reduced parametrization of the inelastic variables using spatially nonuniform fields. To date, the NTFA has been applied to various material models with great success: It enables low number of internal variables, unparalleled compute times and the ability of full field reconstructions during postprocessing.

So far, applications were limited to scenarios where the elastic properties of the material were constant. This is not the case in many situations, e.g., in the presence of distinct temperature changes in metal matrix composites. We present an extension of the NTFA to allow for parametric changes of all thermo-mechanical parameters. This leads to an auxiliary linear elastic reduced order problem that is solved at great efficiency. They allow the computation of the coefficients of the thermo-mechanically coupled NTFA. We demonstrate the outstanding computational performance and the excellent accuary for realistic twoscale problems related to surfaces reinforced by Tungsten Carbide particles

using laser cladding. We believe that our work will be the foundation for future applications including, e.g., damage and fatigue.

Mesh- and model adaptivity for NTFA and full-field elasto-plastic homogenization based on downwind and upwind approximations

Tchomgue Simeu, Arnold; Mahnken, Rolf 08:50
Paderborn University

To increase the quality of computational results for heterogeneous materials like fiber-reinforced composites with Prandtl-Reuss-type material laws, goal-oriented measures of the adaptive finite element method (FEM) coupled to model adaptivity is established. The former is an adaptive mesh refinement on the macroscale, which allows to control the spatial discretization errors. The latter is an efficient combination of a numerically low cost nonuniform transformation field analysis (NTFA) and numerically high cost full-field elasto-plastic homogenization methods on the microscale. The present contribution deals with the application of the concept of downwind and upwind approximations to a goal-oriented a posteriori error estimator based on duality techniques by means of reduced order homogenization schemes like NTFA, and with accuracy and numerical efficiency of the proposed goal-oriented adaptive framework. NTFA consists of an offline phase and an online phase. During the offline phase, some relevant information of the micro system under consideration is precomputed allowing a reduced set of equations to be solved in the online phase. Thus, NTFA leads to a quite efficient homogenization method but less accurate compared to the full-field homogenization method which is characterized with a high computational demand for accounting nonlinear microstructural mechanisms. Due to nonlinearities and time-dependency of 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. Several numerical examples illustrate the effectiveness of the proposed adaptive approach based on downwind and upwind approximations.

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of mean-field and full-field homogenizaton methods in linear elasticity,
Int J Numer Methods Eng, 121(2), 277–307 (2019).

A hyperelastic-plastic mean-field-method at large deformations with damage for CFRP

Zhan, Yingjie; Caylak, Ismail; Mahnken, Rolf 09:10
Paderborn University

Carbon fiber-reinforced plastics (CFRP) are becoming increasingly important due to their outstanding mechanical properties as well as their low weight. In view of the contemporaneous environmental and climate protection policy, there will be a considerable use of CFRP components in the aerospace, automotive and wind energy sector.

Although extensive researches for mean-field-methods have been carried out for physically and geometrically nonlinear problems [1–3], to the author's knowledge, no work exists, which takes into account damage of homogenized CFRP at large deformations. Therefore, this study seeks to develop a mean-field-method for CFRP, that consists of a hyperelastic-plastic matrix with a damage behavior in rate form and hyperelastic fibers with a damage behavior. Moreover, a numerical framework with a fully implicit method for the resulting constitutive relations is proposed.

Finally, two numerical examples are provided, which are compared with experimental data and show the plausibility of the proposed model.

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Parameterized hyperelastic material modeling and multiscale topology optimization with physics-augmented neural network constitutive models

Weeger, Oliver (1); Klein, Dominik K. (1); Roth, Fabian J. (1); Püsch, Felix (1); Maute, Kurt K. (2) 09:30

1: TU Darmstadt
2: University of Colorado Boulder, USA

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 microstructures with parametrized geometry, these materials can be tailored for each specific application. Examples include lattice-metamaterials with varying radii or fiber-reinforced elastomers where the volume fraction of the fibers might vary. Since such materials behave highly nonlinear, their mechanical description is challenging. Thus, we envision the use of physics-augmented neural networks (PANNs), circumventing the current limitations of analytically formulated multiscale material models.

In [1], neural networks are applied to formulate parametrized hyperelastic constitutive models. The models fulfill all common mechanical conditions of hyperelasticity by construction. In particular, partially input convex neural network (pICNN) architectures are applied based on feed-forward neural networks. Receiving two different sets of input arguments, pICNNs are convex in one of them, while for the other, they represent arbitrary relationships, which are not necessarily convex. In this way, the model can fulfill convexity conditions stemming from mechanical considerations without being too restrictive on the functional relationship in additional parameters, which may not necessarily be convex. Two different models are introduced, where one can represent arbitrary functional relationships in the additional parameters, while the other is monotonic in the additional parameters. As a first proof of concept, the model is calibrated to data generated with two differently parametrized analytical potentials, whereby three different pICNN architectures are investigated. In all cases, the proposed model shows excellent performance.

Furthermore, in [2], hyperelastic PANN constitutive models are applied for topology optimization (TO). Using a level-set TO approach, the applicability of hyperelastic PANN constitutive models in 2D and 3D optimization scenarios is demonstrated. The optimized designs received with the PANN constitutive model are in excellent agreement with the ones received with their ground truth counterparts. Furthermore, a parametrized PANN from [1] is applied for multiscale TO. In the optimization process, both the geometry of the macroscale and microstructural parameters are optimized, where the TO with the PANN model again shows excellent results.

[1] D. K. Klein, F. J. Roth, I. Valizadeh, O. Weeger. Parametrized polyconvex hyperelasticity with physics-augmented neural networks. Data-Centric Engineering 4:e25 (2023).

[2] F. Püsch. Nonlinear multiscale topology optimization with material models based on physics-augmented neural networks. Master thesis, TU Darmstadt (2023).

Nonlinear electro-elastic finite element analysis with neural network constitutive models

Klein, Dominik K. (1); Ortigosa, Rogelio (2); Martínez-Frutos, Jesús (2); Weeger, Oliver (1) 09:50
1: TU Darmstadt
2: TU Cartagena, Spain

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 (PANNs), circumventing the current limitations of analytically formulated material models.

In [1], a PANN constitutive model for electro-mechanically coupled material behavior at finite deformations was proposed. 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.

In the present work [2], the applicability of the PANN constitutive model for complex electro-elastic finite element analysis (FEA) is demonstrated. For this, boundary value problems inspired by engineering applications of composite electro-elastic materials are considered. Including large electrically induced deformations and instabilities, such scenarios are particularly challenging, and thus necessitate extensive investigations of the PANN constitutive model. First of all, an excellent prediction quality of the model is required for very general load cases occurring in the simulation. Furthermore, simulation of large deformations and instabilities poses challenges on the stability of the numerical solver, which is closely related to the constitutive model. For the investigations, PANN models are calibrated to different synthetically generated datasets, including data generated with an analytical isotropic potential, a homogenised rank-one laminate, and a homogenised metamaterial with a spherical inclusion. In all cases, the PANN models yield excellent prediction qualities and a stable numerical behavior. This can be traced back to the PANN models excellent performance in learning both the first and second derivatives of the ground truth electro-elastic potentials, even though it is only calibrated on the first derivatives. Overall, this work demonstrates the applicability of PANN constitutive models for the efficient and robust simulation of engineering applications of composite electro-elastic materials.

[1] D. K. Klein, R. Ortigosa, J. Martínez-Frutos, O. Weeger. Finite electro-elasticity with physics-augmented neural networks. CMAME 400:115501 (2022).

[2] D. K. Klein, R. Ortigosa, J. Martínez-Frutos, O. Weeger. Nonlinear electro-elastic finite element analysis with neural network constitutive models. In preparation.

S08.07: FFT and Solver

Date: March 21, 2024 14:00–16:00
Room: G16/054
Chair(s): Waimann, Johanna

A linear algebra perspective on FFT-accelerated finite element solvers for periodic homogenization

Ladecký, Martin (1); Pultarová, Ivana (2); Zeman, Jan (2) 14:00
1: University of Freiburg
2: Czech Technical University in Prague

Introduced to the field of image-based computational micromechanics by Moulinec and Suquet [1], spectral trigonometric solvers have been widely adopted in the field due to their computational efficiency, low memory requirements, and ease of implementation (see [2] for a comprehensive review). In this talk, we focus on the finite element (FE)-based reformulation of the original scheme pioneered by Schneider et al. [3] and Leuschner and Fritzen [4], and (1) provide a linear algebra perspective

on their developments, and (2) relate them to recent advances in Laplace preconditioning of elliptic partial differential equations (e.g., [5]).

Our approach [6] rests on preconditioning the periodic cell problem by a (discrete) Green's operator derived from a reference problem with constant data. On the theoretical side, this implies that the eigenvalues of the preconditioned matrix can be bounded from above and below by coefficients of the original and the reference problem, which means that the system can be solved by the preconditioned conjugate gradient method in a number of steps that is (almost) independent of the grid size. On the implementation side, we exploit the fact that, for a generic arbitrary regular mesh, the system matrix of the preference problem exhibits a block-diagonal structure in the Fourier space and can be efficiently inverted using the Fast Fourier Transform (FFT) techniques. Consequently, the computational complexity of the scheme is dominated by the FFT, making it equivalent to that of spectral solvers. However, in contrast to trigonometric spectral solvers, the proposed scheme works with arbitrary FE shape functions with local supports and does not exhibit the Fourier ringing phenomenon. We conclude the talk by discussing the potential of this framework for controlling discretization and algebraic errors in image-based homogenization solvers.

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FFT-based computational micromechanics with essential boundary conditions

Risthaus, Lennart; Schneider, Matti
University of Duisburg-Essen

14:40

We are concerned with computational multiscale methods which permit reducing the experimental effort to characterize heterogeneous materials significantly. For computational homogenization methods based on the Fast Fourier Transform (FFT), applying periodic boundary conditions is the natural choice [1].
Although applying periodic boundary conditions is suitable for most homogenization problems, alternative boundary conditions may be necessary, e.g. to treat non-periodic porous materials like foams. In this work, we introduce a novel approach to enforce Dirichlet boundary conditions for homogenization problems in solid mechanics and regular grids. By using suitable real FFTs, we retain compatibility with established solvers and software infrastructure [2]. We highlight the computational efficiency of our approach, allowing us to compute effective mechanical properties with Dirichlet boundary conditions on microstructures of industrial scale. We compare the performance of homogenization with non-periodic and periodic boundary conditions and show the influence on computed apparent properties and the agreement with effective properties.

[1] Moulinec H., Suquet P. A fast numerical method for computing the linear and nonlinear mechanical properties of composites, Comptes Rendus de l'Académie des Sciences. Série II, Vol. 318 (11), pp. 1417–1423, 1994.

[2] Schneider M. A review of non-linear FFT-based computational homogenization methods, Acta Mechanica 232, 2051–2100, 2021.

Fourier vs. Radon approach to computational homogenization

Jabs, Lukas; Schneider, Matti
University of Duisburg-Essen

15:00

Since the pioneering work of Moulinec and Suquet, computational methods based on the fast Fourier transform (FFT) have been established as powerful and robust approaches to solve multiscale problems in mechanics. Recently, a similar strategy was proposed by Derraz et al. [1] which utilizes the

Radon transform instead of the FFT for thermal conductivity problems.
In this contribution, we discuss the extension of this new approach to elasticity problems, and investigate the similarities and differences between the two approaches. More precisely, we highlight the common starting point in the continuous setting, and elaborate on the distinguishing features of both approaches, as well as the common features and how they can be leveraged. In particular, the Radon approach permits to view classical FFT-based computational homogenization techniques from a fresh angle. Finally simulation results for microstructures are presented to illustrate and discuss these properties.
References
[1] M. R. Derraz, M. Boukour, A. E. Mamouni, and A. E. Omri, "Three-Dimensional Finite Radon Transform and Linear Homogenization," in Advanced Intelligent Systems for Sustainable Development (AI2SD'2020), pp. 164–182, Springer International Publishing, 2022.

Multiscale(FE-FFT) approach to topology optimization using phase-field methods to generate intentionally designed porous structures

Yaraguntappa, Basavesh; Krischok, Andreas; Keip, Marc-André 15:20
University of Stuttgart

Motivated by cellular materials that are observed in nature and the current capabilities of additive manufacturing methods to fabricate complex designs, which has significantly raised the interest in developing architected cellular materials (ACM) for industrially-relevant high-performance components, in this contribution we propose a multiscale (FE-FFT) approach toward building mechanically optimized ACM's.

We use phase-field methods for topology optimization on two different scales, by combining the inherently mass conserving Cahn-Hilliard phase separation with linear elasticity. On the macro-scale this is solved with 3 field mixed $\mathcal{C}^0$-continuous finite elements (FE) which allows to model an optimized structure with porosity if a smooth interface is chosen whereas on micro-scale (printing scale) a local (periodic RVE) micro-mechanical model is solved using spectral methods (FFT) using the information of macroscopic volume fraction and strain with special triply periodic minimal surface shells as initial microstructures which in the end results in optimal redistribution of the material along and around the direction of the absolute maximum principal strain.

Further aspects that are discussed include improved initial guesses in the macro-scale topology optimization problem and local refinement strategies for the mapping of macroscopic information based on a selective recursive division of cells on the micro-scale.

Finally, some numerical examples are presented to demonstrate the stiffness gain of structures that are modelled with the proposed two-scale framework.

FE-DeepONet: A hybrid solver based on physics-informed deep operator networks for multiscale simulations

Eivazi, Hamidreza; Alikhani, Mahyar; Tröger, Jendrik-Alexander; Wittek, Stefan; Hartmann, Stefan; Rausch, Andreas 15:40
Clausthal University of Technology

Multiscale problems are ubiquitous in physics. Numerical simulations of such problems by solving partial differential equations (PDEs) at high resolution are computationally too expensive for many-query scenarios, e.g., uncertainty quantification, optimization, and control. This limitation has motivated the application of *substitutive* surrogate models, where the micro-scale numerical computations are replaced with a data-driven surrogate, usually acting as a black box mapping between finite-dimensional (discretized) spaces. Substitutive surrogate models are multiple orders of magnitude faster, but purely data-driven substitutive surrogates are generally too data-hungry and inflexible concerning different discretizations or initial and boundary conditions. Moreover, since the micro-scale is completely substituted, the state of the micro-scale is not available when utilizing the surrogate model, and training a physics-informed surrogate by using the governing equations as a constraint is not feasible.

In this contribution, we propose a *complementary*, flexible, and physics-informed learning-based PDE surrogate for the prediction of micro-scale physics by leveraging neural operators. We demonstrate the applicability of our framework for multiscale FE^2 computations, which enable the consideration of the micro-mechanical material structure in macroscopical simulations. In multiscale FE^2-simulations, the microstructure often denoted as a representative volume element (RVE), is also discretized, and the particular initial boundary-value problem is solved using the finite element method. The microstructural responses are usually homogenized quantities, which are then passed to the global macroscopical level. We employ deep operator networks (DeepONets) and formulate a physics-informed operator network to compute approximate solutions for the RVE. Subsequently, homogenized quantities are computed in a manner similar to traditional FE^2 computations, and the consistent tangent operator is obtained using automatic differentiation (AD).

We are the first to combine the FE^2 method with operator learning and develop a hybrid, fast, resolution-independent, and physics-informed approach for multiscale simulations. In this respect, we apply the proposed FE-DeepONet approach to quasi-static problems of solid mechanics. The results demonstrate that FE-DeepONet can yield accurate solutions even when confronted with a restricted dataset during model development. Furthermore, we illustrate that employing an efficient implementation through state-of-the-art high-performance computing libraries and just-in-time compilation can lead to achieving multiple orders of magnitude speed-up.

S08.08: Advanced Numerical and Experimental Techniques

Date: March 21, 2024 17:40–18:40
Room: G16/054
Chair(s): Aldakheel, Fadi

Micromechanics of X-Ray Diffraction Stress Measurements

Krause, Maximilian; Gibmeier, Jens; Böhlke, Thomas 17:40
Karlsruhe Institute of Technology

X-Ray Diffraction (XRD) techniques can be used to measure macroscopic eigenstresses in polycrystalline materials. To interpret measured diffraction patterns as stresses, it is necessary to calculate lattice plane normal strains on the microscale from the macroscopic mean stress. This micromechanical localization problem differs from the usual localization problem in micromechanics since for a given incident beam angle, only particular orientations of grains cause diffraction. Well-established interpretation methods of XRD measurements rely on an ad-hoc choice of the Voigt, Reuss, or Self-Consistent localization approximations [1].
In this talk, existing methods based on these approximations are generalized using the Singular Approximation [2]. In addition, a novel alternative method based on the Maximum Entropy Method [3] is proposed. Both methods depend on a stiffness parameter which can be determined using macroscopic measurements. Instead of an ad-hoc choice of a given localization approximation, this leads to a concrete experimental strategy for choosing the interpretation method most suited to the material.
To validate XRD measurement interpretation methods, a numerical validation strategy is proposed. Using high-resolution full-field simulations based on the fast Fourier transform (FFT), XRD measurements are generated. The number of simulated grains is equivalent to or exceeds common experimental setups. These fully virtual XRD measurements, combined with experimental literature data, lead to quantifiable recommendations for interpretation methods.
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Scale independent extension operators for manifold valued Sobolev maps on perforated domains

Happ, Leon; Gavioli, Chiara; Pagliari, Valerio 18:00
TU Wien

Motivated by *homogenisation problems* in *micro-magnetics and plasticity*, my talk is concerned with the existence of extension operators for Sobolev maps on periodically perforated domains, where the maps are only allowed to range in some prescribed manifold.For applications, one demands that separate L^p bounds for the extension and its gradient, independent of the scale of the perforations, hold. I want to stress that the novelty is really that all functions are subject to a constrained in the target space. The challenge is then to find an extension operator preserving this target manifold constraint**.** Such extension operators prove to be of immense benefit in the field of homogenisation, e.g., for deducing compactness results*.*

Mainly due to Sobolev embeddings, the problem calls for a case differentiation in regard to the relation between the Sobolev exponent p and the dimension n of the domain. The new result I present focuses on the case that p is smaller than n (e.g., in the physically relevant instance that p=2, n=3). Then we can prove the existence of a bounded extension operator for $W^{1,p}$ maps on perforated domains that preserves the described manifold constrained in the target space, under the additional assumption that the target manifold is [p-1] connected. (where [] is the floor function).

The unconstrained case was already treated in an influential paper by E. Acerbi, V. C. Piat, G. Dal Maso, and D. Percivale from 1992, providing a positive answer for all p except infinity. Our work builds upon their result, combining it with an appropriate retraction, firstly suggested by R. Hardt and F.-H. Lin in 1987, and originating from the field of *obstruction theory* in homology. I will present and discuss both ingredients separately; and then, how, by a careful construction, one can derive an extension operator (in the above sense with scale-independent L^p bounds) from them.

I will complete my talk by pointing out how a relaxed version of the extension problem is closely entangled – and even equivalent in some cases – with the question about the surjectivity of the trace operator for Sobolev maps between a manifold with boundary and another target manifold. By studying this relation, it is possible to deduce necessary conditions for the existence of our desired extension operator – also in cases exceeding the assumption of a [p-1] connected target manifold as above.

Application of upper bound rigid-block analysis method to porous solids

Hund, Jonas (1); Kouznetsova, Varvara (2); Alessandretti, Laura (3); Andriollo, Tito (1) 18:20
1: Aarhus University
2: Eindhoven University of Technology
3: Technical University of Denmark

In the realm of modelling heterogeneous solids, two paradigms exist. In micromechanical approaches, the microstructure of such materials is explicitly resolved, aiming to capture morphology, distribution, and material properties of each phase. Due to their resolution, micromechanical methods are computationally expensive and usually limited to the microscale. For investigations of macroscopic parts made from a heterogeneous material at reasonable expense, homogenisation methods are used. However, due to capturing the material's microstructure only in a macroscopic manner, these approaches' capabilities in resolving non-uniform material properties, e.g. due to the distribution of phases, and related localisation phenomena are limited. Experimental studies have revealed that deformation in porous solids or heterogeneous solids with soft inclusions localises in so-called shear bands that spawn in between voids or particles, respectively, and constitute zones where energy is dissipated through plastic deformation. Due to the associated computational costs, prediction of strain localisation in and macroscopic strength of porous solids, particularly with non-uniformly distributed voids, remains a challenge. In this contribution, the aim is to assess the load limit of representations of 2D random microstructures with a given porosity through an upper-bound limit analysis method at significantly reduced computational cost compared to other micromechanical approaches.

The model domain is discretised using rigid elements, restraining all deformation and energy dissipation to sliding and inner friction along discontinuities introduced at element boundaries. Hence, the shear bands as narrow zones of strain localisation and plastic dissipation are modelled through discrete lines that constitute discontinuities of the velocity field within the model domain. Previous work of the authors established that the Delaunay triangulation of the considered microstructures features edges that coincide with the locations of shear bands when the void centroids serve as the nodal grid. Based on this finding, the model domain is discretised using Delaunay triangulation allowing for an efficient and effective reduction of the number of potential discontinuities further lowering the computational cost of the rigid block sliding mechanism presented. To demonstrate the method's capabilities, predicted limit loads under uniaxial tension and deformation patterns in representations of random periodic microstructures are compared to results from a finite element study.

S08.09: Material Modeling

Date: March 22, 2024 08:30–10:30
Room: G16/054
Chair(s): Langenfeld, Kai

Concepts for modeling the inelastic behavior of foam structures

Abendroth, Martin; Malik, Alexander; Kiefer, Bjoern
TU Bergakademie Freiberg
08:30

The presentation compares two approaches for modeling the inelastic behavior of foam structures. The first approach is classical in nature, where analytical representations for the yield surface and the yield potential are used in a thermodynamically consistent modeling concept. The difficulty here is to formulate the analytical approaches. By adapting the formulation for a yield surface by Ehlers, which was originally developed for geomaterials, a very good agreement with numerically determined yield surfaces could be achieved. The parameters of the analytical yield surface can be represented as functions depending on a hardening variable. The second approach is purely data-driven and uses approximations such as bivariate splines or neural networks for the representation of yield surface and yield potential. The neural networks used are so-called feed-forward networks and are used as universal approximators or regressors. The data required for the training are obtained from finite element simulations of representative volume elements of generic foam structures, whereby the stress-controlled load paths are systematically varied. The approaches used are compared in terms of their suitability, flexibility and accuracy for describing the inelastic behavior of foam structures.

Multiscale analysis of interlocking effects for polymer additive manufacturing on aluminum foam

Timmann, Frederic; Gronwald, Paul-Luis; Hürkamp, André; Dröder, Klaus
TU Braunschweig
08:50

This study examines a novel approach for manufacturing hybrid functional structures, combining extruded aluminum profiles and additive-manufactured thermoplastic structures. The non-assembly approach aims to print the functional structures directly onto the surface of the aluminum profile using local, near-surface applied aluminum foam structures for mechanical interlocking. For this purpose, the closed-cell aluminum foams require open pores on the surface. The filling of pores in the aluminum foam with the polymer affects the bond strength of this hybrid compound. Within a simulation-based process design the additive manufacturing process parameters are investigated using a computational fluid dynamics (CFD) model with fluid-structure interaction (FSI) for the pore-filling process and a finite element model to evaluate the resulting bond strength. The material throughput, the nozzle distance, the polymer, and the substrate temperature are the key process parameters taken into account. Virtual foam models are used within this framework, where a linear movement of the extruder nozzle and the resulting polymer strand is investigated. A criterion is defined to determine the optimal pore filling and strand width to prevent over-extrusion and the closure of adjacent

pores. This method includes the mesh conversion from the CFD results to the FEM mesh for structural analysis by exporting the iso-surface for the polymer strand geometry embedded in the pores of the aluminum foam structure.

FE^2 method to model plane and rod-like carbon-based nanostructures

Ochs, Julian; Wackerfuß, Jens
University of Kassel

09:10

Due to their excellent mechanical, electronic and chemical properties, carbon-based nanostructures have great application potential in electronic devices such as transistors and solar cells. If local effects such as vacancy defects and bond breaking or making scenarios play a role in such structures, a numerical simulation must be carried out within the framework of molecular dynamics [1]. However, as this becomes inefficient for very large nanostructures, multiscale models are developed and used. In this context, a general distinction is made between sequential and concurrent multiscale methods.

In our presentation we will focus on the FE^2 approach, which belongs to the category of concurrent multiscale methods (there in the subcategory 'hierarchical approach'). While a continuum model is used at the macro level, an atomistic model is used at the micro level. The methods presented in the literature use molecular dynamics at the micro level; suitable coupling strategies have been developed for the scale transition. In contrast, we restrict ourselves to static problems and use the homogenization process presented by Miehe and Koch [2]. Specifically, 2 models are presented: a) for modeling planar nanostructures (such as graphene) we use a plane continuum model on the macro level and b) for rod-like nanostructures we use a beam model. In both cases, the atomistic model is implemented at the micro level in the context of FEM [3, 4]. Different boundary conditions to be applied to the RVE, which fulfill the Hill-Mandel condition [5], are compared with each other; in particular with regard to their independence with respect to the size of the RVE. The presented multiscale model is validated by means of fully atomic simulations. In addition, a comparison with simulations based on the Cauchy-Born rule is made in terms of efficiency, accuracy and implementation effort.

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FE^2 simulation of low-cycle fatigue in metals

Zobel, Maximilian (1); Hütter, Geralf (1,2)
1: BTU Cottbus-Senftenberg
2: TU Bergakademie Freiberg

09:30

Low-cycle fatigue is a highly relevant aspect in assessing a structures durability. In the realm of low-cycle fatigue in metallic structures, microscopic damaging and redistribution of macroscopic stresses due to cyclic plasticity interact complexly. This complexity is heightened in non-proportional loading and stress-concentrated regions like notches. Rather than tackling the challenge of developing phenomenological models for these intricate effects, the study opts for a multi-scale approach. Employing scale bridging techniques, it transfers processes of plasticity and damage accumulation from the microstructure to the structural scale. This contribution utilizes and compares FE^2 technique and

reduced order modelling for multi-scale simulations, specifically addressing the cyclic growth of microvoids in notched components subjected to nonhomogeneous loading conditions. It further highlights the evaluation of various numerical techniques aimed at maintaining a manageable computational effort, and the predictions from the simulations are systematically compared with corresponding experimental data.

Modeling microstructural effects in scaffold mediated bone regeneration

Dondl, Patrick; Suchan, Oliver
University of Freiburg

09:50

When bone defects of large size occur, also called critical defects, the regenerating bone tissue is not able to bridge the resulting gap on its own and an additional artificial structure is necessary to support bone growth. We present a general framework to phenomenologically model the growth of bone mediated by such a scaffolding structure. The microstructural geometry and the porosity of the implemented structure have a significant impact on the bone growth rate which we seek to maximize by means of PDE constrained optimization. To also account for the microstructure we use periodic homogenization at each point of the macro space. Implemented within the firedrake framework, ExternalOperators enable us to perform this micro-macro coupling with differing approaches for solving the micro and macro problems respectively. Here, we present the classical FE^2-method and compare it to a faster FE-FFT-approach.

S09: Laminar flows and transition

Organizer(s): Wünsch, Olaf *(University of Kassel)*

S09.01: Various topics in Laminar flows and transition

Date: March 19, 2024 08:30–10:30
Room: G22/216
Chair(s): Wünsch, Olaf

Application and parameter identification of the Lagrangian-averaged vorticity deviation vortex detection method in three-dimensional flows around solid bodies

Kovács, Kinga Andrea; Balla, Esztella 08:30
Budapest University of Technology and Economics

The flow around different objects has been intensively studied due to its wide-ranging practical applications. Vortices around solid bodies may cause vibration and noise, making their occurrence undesirable. The risk intensifies when the frequency of vortex shedding aligns with the natural frequencies of the bodies. Therefore, engineers must consider vortex shedding effects during the design of structures such as skyscrapers and chimneys to mitigate potential risks. A thorough investigation of vortex structures is required to identify vortices, quantify their impact, and construct mitigation plans.

A promising vortex detection technique is the Lagrangian-averaged vorticity deviation (LAVD) [1]. The calculation of the LAVD values includes the integral of vorticity along particle trajectories. This technique can detect the center and the boundary of vortices. Important parameters of the method include the size of the sought vortices and their convexity. The authors aim to provide recommendations for these parameters based on previous 2D [2] and current 3D simulations of vortex rows behind cylinders, serving as simplified models for skyscrapers and chimneys.

The appropriateness of the method for the detection of vortex rows behind bluff bodies is proven by the identification of the von Karman vortex street, which is characterized by symmetric and periodic vortex shedding. The locations of the detected vortex cores are in accordance with the theoretical values. Laminar simulations are performed with the help of ANSYS Fluent, and the vortex detection is carried out in MATLAB.

The capabilities of the LAVD technique are also tested on a practical example of a flow around an axial fan. The so-called tip leakage vortex (TLV) is in the focus of the simulations (obtained with the RANS SST k-ωmodel) because it may cause losses and noise in small-scale axial fans. The results show that the LAVD method is able to detect vortical structures around the blades of turbomachines.

The novelty of the above research can be summarized as follows:

a) Recommendation for the parameters of the LAVD technique

b) 3D implementation of the LAVD technique for flows containing solid bodies

c) Application of the LAVD technique for turbomachinery

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Energy stability analysis of MHD flow in a rectangular duct

Boeck, Thomas (1); Brynjell-Rahkola, Mattias (1); Duguet, Yohann (2) 08:50
1: TU Ilmenau
2: LISN-CNRS, Université Paris Saclay

The behavior of perturbations imposed on laminar shear flows plays a crucial role for the understanding of transition to turbulence. Instability of infinitesimal perturbations, i.e. linear instability, ensures

that the laminar state cannot be maintained at a given Reynolds number. However, wall-bounded shear flows exhibit turbulence for Reynolds numbers well below the critical Reynolds number for linear instability. Energy stability analysis provides a lower bound for the Reynolds numbers where non-laminar flow can persist. Like linear instability analysis, it results in a linear eigenvalue problem. We study the energy stability of electrically conducting flows in a rectangular duct with transverse homogeneous magnetic field and electrically insulating walls. For sufficiently strong fields, the laminar velocity distribution of these MHD duct flows has a uniform core and Hartmann and Shercliff boundary layers on the walls perpendicular and parallel to the imposed magnetic field. The thickness of these layers depends on the Hartmann number as nondimensional parameter for the strength of the magnetic field. The MHD duct flows also exhibit turbulence for parameters well below their linear stability limits. For the energy stability analysis we employ a spectral discretization by a double expansion in Chebyshev polynomials in the cross-stream coordinates. The eigenvalue problem for the critical Reynolds number depends on the streamwise wavenumber, Hartmann number and the duct aspect ratio. We consider small and large aspect ratios in order to compare with stability models based on one-dimensional approximations of the base flows. For large aspect ratios we find good numerical agreement with the quasi-two-dimensional approximation. The lift-up mechanism dominates for small streamwise wavenumbers and provides a linear dependence between the critical Reynolds and Hartmann number in the duct. The duct results for small aspect ratio converge to Orr's original energy stability result for spanwise uniform perturbations imposed on the plane Poiseuille base flow. We also examine the different symmetries of eigenmodes.

Modeling active suspensions with the mixture theory

Ben Gozlen, Houssem; Wang, Yongqi; Oberlack, Martin 09:10
TU Darmstadt

We model an active suspension using the mixture theory [1]. The suspension consists of a linear viscous liquid infused with a large number of identical active particles. The focus of the present work is on modeling the stress tensor of the particle phase and the interaction force between the fluid and particle phases. 1D-shear flows driven by the active force of the particles and/or a pressure gradient are firstly investigated. Depending on the magnitude and direction of the active force and the pressure gradient, the particles can condensate in the center of the channel or on the wall. Then the flow of an active suspension in an annular channel with a rectangular cross-section is solved numerically. A stable secondary flow pattern emerges in the cross-section of the channel. It consists of structures that are similar to the Taylor-Couette instability[2]. The effect of the Dean Number and the aspect ratio of the cross-section on the secondary flow are investigated. The physical quantities of interest e.g. the volume fraction and partial velocities of both phases are discussed.

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S10: Turbulence and reactive flows

Organizer(s): Janiga, Gabor *(University of Magdeburg)*
Voß, Samuel *(University of Magdeburg, Otto-von-Guericke)*

S10.01: Various topics in Turbulence and reactive flows

Date: March 20, 2024 08:30–09:30
Room: G22/216
Chair(s): Janiga, Gabor

Stochastic modeling of a turbulent hydrogen/nitrogen jet flame in a vitiated coflow

Starick, Tommy; Schmidt, Heiko 08:30
BTU Cottbus-Senftenberg

This preliminary numerical study investigates a lifted hydrogen/nitrogen jet flame in a vitiated coflow by means of the map-based, stochastic one-dimensional turbulence (ODT) model. The ODT model is affordable in terms of computational costs and provides nonetheless full-scale resolution along a notional line of sight crossing the turbulent flow field. In the considered Cabra burner configuration [Proc. Combust. Inst. 29/2 1881-1888 (2002)], a turbulent jet flame of hydrogen/nitrogen (Re=23,600, H/d=10) issues from a central nozzle into a vitiated coflow of hot combustion products generated from an array of lean hydrogen/air flames (T=1045K). Centerline and radial profiles for mixture fraction, temperature and species mass fractions obtained from ODT simulations using a reduced reaction mechanism are compared to experimental measurements of Cabra et. al.. Two-dimensional visualizations of the vitiated coflow burner are also provided. Vitiated coflow burners exhibit similar characteristics for chemical kinetics, heat transfer and molecular transport as recirculation burners in advanced combustors. The subtle interactions of the hot coflow with the cold unburnt jet flow are crucial for the entire reaction and autoignition process of the jet. Considering the reduced order and efficiency of the model, ODT is a suitable tool for extensive parameter studies without compromising on the full resolution of all relevant length and time scales. In the talk, we will additionally present scatter plots of temperature and OH mass fraction and examine the dependence of the liftoff height on the coflow velocity.

Optimising production of synthetic natural gas (SNG) from methane synthesis

Rakhi, Rakhi; Mauss, Fabian 08:50
BTU Cottbus-Senftenberg

To optimise the methanation of synthesis gas (syngas) with a focus on achieving maximum methane and minimum CO, a comprehensive thermodynamics analysis of CO_2 hydrogenation is conducted. This study will help us to understand the thermodynamic behaviour of the reactions involved in methanation process. We have investigated the species, CO_2, H_2, CH_4, H_2O, and CO at the equilibrium in a temperature range of 200-1200 °C with pressure variation of 1 atm to 300 atm and a fuel composition of H_2/CO_2 ratio of 2 to 6. Low temperatures (200-400 °C) and high pressures are favourable for the consumption of CO_2 and H_2 as well as to obtain maximum CH_4. Also, in this temperature range, there is no carbon formation. Higher H_2/CO_2 ratio favours CO_2 consumption but influence CH_4 formation. Trace amount of O_2 in syngas is unfavourable for methanation and additional CH_4 is favourable. The carbon formation is a serious issue that starts around 400 °C and above, for all the fuel compositions at 1 atm. This can be shifted to slightly higher temperatures, i.e., 600 °C if high pressures are selected. The study can help us to select the optimum conditions (temperature, pressure, and H_2/CO_2 ratio) to perform the experiments to achieve maximum CH_4 by full methanation of CO_2 avoiding the carbon formation issue. This will also support us for the development of catalysts and processes for the production of natural gas which can be reintegrated into the network of natural gas.

Detached eddy simulation (DES) of a turbulent premixed flame stabilized on a bluff body

HEMAIZIA, Abdelkader (1); Thévenin, Dominique (2); Chi, Cheng (2)
1: University of Science and Technology – Houari Boumediene, Algeria
2: Otto von Guericke University Magdeburg

09:10

The design of future combustion chambers increasingly relies on numerical simulations. Detached eddy simulation (DES) emerged as a method that offers a higher predictability for turbulent flames compared to Reynolds-averaged Navier-Stokes (RANS) approaches in reacting flows. This work describes an investigation based on DES to analyze a premixed burner equipped with a bluff body. The turbulence-chemistry interaction scheme is treated using the Eddy Dissipation Concept (EDC) model in combination with a skeletal mechanism. Three different reduced reaction mechanisms, for propane-air, methanol-air, and hydrogen-air, are investigated using the industrial code ANSYS-Fluent and compared in this study. For each case, simulations are performed using a structured non-uniform grid refined in high gradient area. Experimental data from the reference, so-called Volvo combustor are used for validation of two baseline cases (Case A and B), described in Table 1.

Table 1: Considered parameter for the two cases, A and B.

Case | T_0 (K) | P_0 (atm) | m_0 (kg/s) | Φ | v_0 (m/s) | Re_0 |

A | 288 | 1.0 | 0.60 | 0.62 | 17.6 | 46.592 |

B | 600 | 1.0 | 0.60 | 0.62 | 36.6 | 27.629 |

S10.02: Various topics in Turbulence and reactive flows

Date: March 20, 2024 14:00–16:00
Room: G22/216
Chair(s): Janiga, Gabor

Numerical studies in compressible thermal convection flows

Panickacheril John, John; Schumacher, Jörg
TU Ilmenau

14:00

Buoyancy-driven turbulent convection leads to a fully compressible flow with a prominent top-down asymmetry of first- and second-order statistics when the adiabatic equilibrium profiles of temperature, density and pressure change very strongly across the convection layer. The growth of this asymmetry and the formation of an increasingly thicker stabilized sublayer with a slightly negative mean convective heat flux at the top of the thermal convection zone is reported here by a series of highly resolved three-dimensional direct numerical simulations (DNS) which apply a compact finite difference method. These DNS are conducted beyond the Oberbeck–Boussinesq and anelastic limits for dimensionless dissipation numbers, $0.1 \leq D \leq 0.8$, at fixed Rayleigh number Ra = 1e+6 and a superadiabaticity ε= 0.1. The dissipation number D determines the degree of stratification in the convection layer. The highly stratified compressible convection regime appears for $D > Dcrit$ 0.65, when density fluctuations collapse to those of pressure; it is characterized by an up to nearly 50 % reduced global turbulent heat transfer and a sparse network of focused thin and sheet-like thermal plumes falling through the top sublayer deep into the bulk. We discuss the connections between statistics and structures in the flow and connect our study to potential applications in natural convection flows.

Numerical Study on the Effects of Transient Pressure Gradients on Isothermal and Heated Pipe Flows

Polasanapalli, Sai Ravi Gupta; Klein, Marten; Schmidt, Heiko
BTU Cottbus-Senftenberg

14:20

Flow inside heated pipes is common in both industrial and domestic uses. Besides natural gas, also heat (warm water) is transported via pipelines and into the ground for geothermal applications. The latter involves borehole heat exchangers for geothermal storage. In these facilities, there is an application of canonical heated pipe flow. Efficiency, that is, economical operation, is crucial and depends on

optimizing heat transfer and pressure loss properties. The latter is a consequence of frictional losses in the fluid flow and governs the required pumping power. The flow is desired to be turbulent if heat transfer is to be increased, which leads to higher frictional losses than in the laminar regime. Many methods, such as surface modifications, polymer additions to fluids, and relaminarization, have been suggested to reduce the drag, but these are impractical for the mentioned applications. In two recent studies [1, 2], pulsatile driving of pipe flows with transient pressure gradients and cardiac-cycle-like waveforms was shown to reduce turbulence drag and hence improve energy efficiency. This method operates pumps in a transient manner as opposed to altering fluid characteristics and wall properties.

The present study aims to explore the impact of transient pressure gradients on flow drag and heat transfer properties at moderately high Prandtl number and high Reynolds numbers not reached previously. While reducing pressure drag is advantageous, heat transfer rates are critical for geothermal heat exchangers. Here, three-dimensional numerical simulations will be conducted using an off-lattice Boltzmann method solver [3] in combination with a standalone map-based stochastic turbulence model [4] for parametric extrapolation. In the talk, the first results from both approaches will be shown, focusing on forced convection with transient forcing.

References:

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Stochastic modeling and theoretical analysis of heated concentric coaxial pipes at low Prandtl number

Tsai, Pei-Yun; Schmidt, Heiko; Klein, Marten 14:40
BTU Cottbus-Senftenberg

Concentric coaxial pipe flows play an essential role in the engineering sector, such as heat exchangers, heated pipes, and chemical reactors. Heated concentric pipes have been studied previously only for low Reynolds numbers to investigate the dependence of radius ratio [1] and thermal boundary conditions [2]. However, an accurate but economical approach to acquire robust predictions of both heat transfer and pressure loss at high Reynolds number and low Prandtl number has remained a challenge for state-of-the-art numerical methods and turbulence models. Reduced-order stochastic modeling, here by means of the so-called one-dimensional turbulence model [3] (ODT), is able to address this challenge as demonstrated previously [4, 5]. This is achieved by modeling turbulent eddies through a stochastically sampled sequence of physical mapping events that punctuate the continuous (molecular-diffusive) flow evolution. The formulation adopts an instantaneous interpretation of mixing-length phenomenology. This is known as map-based advection modeling. Still, a careful investigation of the scaling properties of the statistical moments of fluctuating flow profiles and of the heat transfer has not been done. In this study, we investigate the turbulent flow in pressure-driven concentric coaxial pipes with momentum and passive scalar transfer using the ODT model to reach high Reynolds and low Prandtl numbers. In the contribution, we demonstrate that results from the stochastic model are consistent with mixing length theory. By extending available boundary layer theory to spanwise curvature for heat transfer, we discuss how the wall-curvature related asymmetry of the thermal boundary layer over the cylindrical inner and outer wall emerges. The latter induces Reynolds and Prandtl number dependencies.

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Measurement of active grid generated turbulence

Szaszák, Norbert; Bencs, Péter
University of Miskolc, Hungary

15:20

The aim of the research is the investigation of the flow field downstream of an active turbulence grid using LDA and CTA measurement methods. The work includes the development of measurement cases, the designing and realization of the measurement and auxiliary systems.

The investigation has been realized in a Göttingen-type wind tunnel in its open-mode, with a measurement cross section of 0.6 x 0.5 m. The investigated grid type active turbulence generator was placed downstream of the converging nozzle section of the wind tunnel. Flexible silicone tubes were attached to certain grid points of the turbulence generator. Based on previous experiment results, silicone tubes were placed at every second grid point in a checkerboard pattern, and the remaining grid point openings were closed. In active and in jet modes of the grid, it was supplied with auxiliary air of up to 8 bars, which was adjusted to the appropriate volume flow with the help of a pressure reducer and a variable cross-section volume flow meter.

The flow downstream of the turbulence grid was examined at five different mean air velocities with the turbulence generator was operated in passive, jet and active modes. The Reynolds numbers, the mass flow ratio of the auxiliary air and the main flow relative to each other, as well as the units of measurement required for their determination (such as viscosity, density etc.), were determined. In the case of LDA measurements, the vertical component and horizontal main direction velocity component (u-w) were measured. During the CTA measurements, the measurements were performed twice, once measuring the horizontal main direction and the horizontal velocity component perpendicular to it (u-v), and the second time measuring the horizontal main direction and the vertical component perpendicular to it (u-w). The results were processed and visualized using Matlab.

S11: Interfacial flows

Organizer(s): Fricke, Mathis *(TU Darmstadt)*
Maric, Tomislav *(TU Darmstadt)*

S11.01: Interfacial Transport, Mass Transfer and Flow Instabilities

Date: March 20, 2024 16:30–18:30
Room: G22/216
Chair(s): Fricke, Mathis
Maric, Tomislav

Modeling and Simulation of Simultaneous Transport and Incompressible Flows on all Level Sets in a Bulk Domain

Fries, Thomas-Peter; Kaiser, Michael Wolfgang 16:30
Graz University of Technology

Flows and transport processes on curved manifolds embedded in some higher-dimensional background space have recently gained significant interest [1, 2]. In most cases, two-dimensional surfaces/interfaces in the three-dimensional space are considered. Herein, instead of only focusing on processes on *one* surface, infinitely many surfaces are considered *at once*. Starting point is a higher-dimensional bulk domain and a level-set function. The level sets imply infinitely many manifolds with co-dimension one. That is, for three-dimensional bulk domains, the level-set function implies a set of curved two-dimensional surfaces. Mechanical models for heat flow (transport), Stokes flow and incompressible Navier-Stokes flows are formulated *simultaneously* on all level sets. A numerical method, recently coined the Bulk Trace FEM [3], is applied for the simulation. Therefore, the bulk domain is discretized by higher-order background elements, conforming to the boundary of the bulk domain. However, these elements do not conform to the shape of the level sets, so that it may be seen as a hybrid between the classical, conforming Surface FEM and the non-conforming Trace FEM [4]. However, the Bulk Trace FEM does not come with the usual challenges of the Trace FEM with respect to integration, boundary conditions, and stabilization. These issues are all conveniently treated as usual for the Surface FEM. Numerical results confirm the success of the proposed simultaneous models and the Bulk Trace FEM in various contexts, even enabling optimal, higher-order accurate results when smooth solutions are expected.

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Unstructured Finite-Volume Arbitrary Lagrangian / Eulerian Interface Tracking computational framework for incompressible two-phase flows with surfactants

Schwarzmeier, Moritz (1); Raju, Suraj (1); Tukovic, Zeljko (2); Fricke, Mathis (1); Bothe, Dieter (1); Maric, Tomislav (1) 17:10
1: TU Darmstadt
2: University of Zagreb, Croatia

We present an open-source computational framework that implements the unstructured Finite-Volume Arbitrary Lagrangian / Eulerian (ALE) Interface Tracking method for incompressible two-phase flows with surfactants.

The framework implements the Interface Tracking ALE method for incompressible two-phase flows using a segregated solution algorithm for solving coupled Navier-Stokes equations with interfacial

jump conditions. The Finite Area method discretizes transport equations on curved and evolving fluid interfaces. The open-source implementation as an OpenFOAM module also contains the Sub-Grid-Scale (SGS) model for handling extremely narrow boundary layers of passively transported scalars with very small diffusivity.

The SGS model significantly reduces resolution requirements for species transport across the fluid interface. The surface and bulk transport of surfactants and the SGS model are verified using (semi-)analytical verification cases. We also discuss complex setups, e.g., of a rising bubble at high Peclet-numbers under the influence of soluble surfactants.

hp-Adaptive Simulation of Compressible Two-Phase Flows with Phase Transition

Mossier, Pascal; Munz, Claus-Dieter; Beck, Andrea D. 17:30
University of Stuttgart

The process of phase transition is a defining characteristic of interfacial flows and at the heart of fundamental environmental processes like the water cycle. In engineering, the understanding and reliable prediction of interfacial flows with phase transition is essential for current and future propulsion systems of airliners and orbital launch systems. Here, an efficient vaporization and mixing of carbon-based fuels and the upcoming e-fuels is vital to achieve a stable and complete combustion and thus reduce the emission of greenhouse gases.

However, the development of numerical models and simulation me1thods to provide high-fidelity simulations for such processes is still subject of ongoing research. A key challenge hereby is the multi-scale character of the underlying problem: While the flow field can be described by macroscopic continuum models, the interface dynamics during phase transition are driven by microscopic interactions on a molecular level. Further, the flow field itself poses a multi-scale problem when turbulent structures appear in the bulk flow. Finally, under extreme ambient conditions, compressible effects cannot be neglected and force a tight coupling between the hydrodynamics and interface local thermodynamics as well as a careful treatment of shocks in the flow field.

To address these challenges, the talk focuses on a sharp-interface-based methodology, developed for the simulation of compressible two-phase flows with phase transition. It relies on a highly efficient hp-adaptive hybrid Discontinuous Galerkin and Finite Volume scheme to cope with the various scales in the bulk flow and to achieve an accurate interface localization. The hybrid operator combines the high-order accuracy of the DG method and the robustness of the FV scheme and applies p-adaptation in smooth areas and h-refinement at discontinuities. To tackle the multi-scale problem at the phase boundary, the method relies on a two-phase Riemann solver to incorporate interface-local thermodynamics through a microscopic evaporation model. It is based on a hyperbolic description of heat conduction and derived with non-equilibrium thermodynamics to provide coupling of the bulk phases at the phase boundary.

The accuracy and efficiency of the proposed hp-adaptive sharp-interface method is demonstrated with challenging multi-phase problems involving complex shock patterns, severe interface deformations and merging interface contours. Further, the developed interfacial Riemann solvers are validated against molecular dynamics data. Finally, the combined framework is applied to simulate a shock-droplet interaction with phase transition in full three dimensions.

Simultaneous experimental analysis of concentration and velocity fields in gravity-driven inclined liquid film flows over smooth and microstructured surfaces

Weigelt, Johann; Brösigke, Georg; Repke, Jens-Uwe 17:50
TU Berlin

Within chemical industry, thermal separation processes play a significant role in the treatment of fluid mixtures. Structured packings are essential in columns for absorption and rectification processes. The separation efficiency of packing columns depends on the interaction between the gaseous and liquid phases within the packing elements, making the optimal selection of packing geometry necessary. The characteristic geometry of structured packings, defined by macro- and microstructures,

enables to achieve a maximized interfacial area for mass transfer and homogeneous gas distribution with minimal pressure drop.

Microstructures, ranging from several hundred micrometers to millimeters, significantly influences the performance of packing columns. Fundamental experimental studies on inclined plate elements in laboratory scale by Kohrt et al. (2011) reveal a substantial enhancement in mass transport due to microstructures, with fluid dynamic phenomena assumed to be the cause, resulting from the interaction of liquid flow with the microstructure. However, the specific mechanisms by which microstructures influence momentum distribution and subsequently affect mass transport within liquid laminar film flows are not fully investigated.

The objective of this study is to simultaneously analyze local velocity and concentration distributions in laminar liquid film flows (Re < 40) within the influence region of 2D and 3D overflowed microstructures during gas absorption. The influence of locally induced velocity distribution by microstructures on local mass transfer will be directly investigated experimentally. The concentration field is measured using a planar laser-induced fluorescence (PLIF & PLIF-I) method, while simultaneously measuring the velocity field using a stereo particle image velocimetry (SPIV) method. Both methods have been successfully modified and applied separately for film flows (Gerke and Repke 2019, Bonart et al. 2017).

This research compares the characteristics of gravity-driven inclined laminar film flow on a smooth plate and a 2D structured plate. The ratio of the Nusselt film height to the structure height is maintained at values below 1 and the observation focuses on a localized point of view within the range of 5 x 5 mm. Optical non-invasive measurements have been carried out in a steady state, focusing on determining the mass transfer into a viscose mixture of glycerol and water. Two oxygen sensitive dyes consisting of ruthenium (PLIF-I) and resorufin (PLIF) are applied to measure the concentration fields. The theoretical analytical solution for a smooth plate will be utilized to validate the setup. For this process, the diffusion coefficient will be determined using the methodology proposed by Jimenez et al. (2012).

Capabilities and limitations of Smoothed Particle Hydrodynamics for the simulation of two-phase flow instabilities

Vallem, Rishindra (1,2); Klein, Marten (1,2); Schmidt, Heiko (1,2) 18:10
1: BTU Cottbus-Senftenberg
2: Scientific Computing Lab, Energy Innovation Centre, Cottbus

Two phase internal flows are encountered in many engineering applications and result in various flow regimes such as stratified flow, wavy flow, elongated bubble flow, and slug flow. Slug flow, among these, is of high interest because of its intermittent nature and associated vigorous fluctuations in mass flow rate and pressure, which needs to be avoided in technical flows. Smoothed Particle Hydrodynamics (SPH) is a mesh-free, Lagrangian particle-based computational fluid dynamics (CFD) tool that is able to simulate dispersed multiphase flows in an economical manner. However, the capabilities for capturing flow regimes and regime transitions, among numerical convergence, is not yet generally established. In this work, two solvers, a commercial solver (PreonLab) and an open-source solver (DualSPHysics), are evaluated for their off-the-shelf capabilities to model canonical nondispersed two-phase flows as summarized below.

First, a laminar rising bubble case is considered in order to evaluate the fluid-fluid interface representation and transient interface evolution. This requires a physics-compatible modeling of surface tension, buoyancy, and viscous effects. While both solvers used are able to yield qualitatively reasonable predictions, PreonLab proved to be more accurate comparatively and also showed much better agreement both qualitatively and quantitatively with the chosen reference data.

Second, the Kelvin-Helmholtz Instability (KHI) is investigated using PreonLab. The KHI provides a key mechanism for the onset of flow regime transitions, in particular, from stratified flow to slug flow. An idealized case and a complex case is considered. The idealized case is shear-dominated with gravity and surface tension effects neglected. A low density ratio (1:2) is assumed. The complex case includes surface tension and gravity and assumes a high density ratio (1:800). KHI exhibits a linear and a nonlinear growth regime. The linear growth rate is up to 50% lower in present SPH simulations than in the

prediction by Linear Stability Theory (LST). While some other numerical studies have reported deviations of similar order for pseudo-spectral and SPH-based approaches, the reason for this deviation is not yet clear. In the nonlinear regime, by contrast, the expected mixing-layer similarity is reproduced well. For the complex case, the numerically estimated stability margin was found to reasonably match the theoretical prediction.

S11.02: Analytical and Numerical Methods for Two-Phase Flows

Date: March 21, 2024 08:30–10:30
Room: G22/216
Chair(s): Fricke, Mathis
Soga, Kohei
Maric, Tomislav

Mathematical analysis of modified level-set equations

Soga, Kohei (1); Bothe, Dieter (2); Fricke, Mathis (2) 08:30
1: Keio University, Japan
2: TU Darmstadt

The linear transport equation allows to advect level-set functions to represent moving sharp interfaces in multiphase flows as zero level-sets, where the equation in this context is particularly called the level-set equation. A recent development in computational fluid dynamics is to modify the level-set equation by introducing a nonlinear term to guarantee the norm of the gradient of the level-set function to be a priori bounded, where the zero level-set must be unchanged by the modification. This leads to more accurate approximation of the interface normal, mean curvature, etc. Unlike reinitialization methods, the nonlinear modification technique combines the advection of the interface and the control of the norm of the gradient into one single PDE. It is important to note that, due to the nonlinear term, the modified level-set equation is a first order fully nonlinear PDE, where existence of a classical solution on the whole domain within an arbitrary time interval is no longer possible in general and a notion of weak solutions is required for wellposedness.

The present work establishes mathematical justification for a specific class of modified level-set equations on a bounded domain, generated by a given smooth velocity field in the framework of the initial/boundary value problem of Hamilton-Jacobi equations. The first result is the existence of smooth solutions defined in a time-global tubular neighborhood of the zero level-set, where an infinite iteration of the method of characteristics within a fixed small time interval is demonstrated; the (local in space) smooth solution is shown to possess the desired geometrical feature. The second result is the existence of time-global viscosity solutions defined in the whole domain, where standard Perron's method and the comparison principle are exploited. In the first and second results, the zero level-set is shown to be identical with the original one. The third result is that the (merely continuous) viscosity solution coincides with the local-in-space smooth solution in a time-global tubular neighborhood of the zero level-set. This result is relevant both from a PDE and an application point of view: it provides a new technique of local comparison between a viscosity and a classical solution, yielding partial regularity of viscosity solution; it justifies the use of numerical methods on the whole domain in the class of viscosity solutions, still providing well-defined interface normal and mean curvature, while numerical construction of the local-in-space classical solution seems much more challenging.

Two-Phase Flow Simulations in a Space-Time Framework for Injection Molding Applications

Ferrer Fabón, Blanca; Behr, Marek 09:10
RWTH Aachen University

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 present a macro-scale two-phase flow formulation for polymer injection molding. We use an in-house finite-element solver to simulate the polymer and air flows as an interfacial flow, utilizing the level-set method in a space-time framework. For a high-fidelity simulation, complex material models are introduced to represent the melted polymer, i.e., shear-thinning viscosity, crystallization, pvT model, and other temperature-dependent properties. We discuss the numerical treatment of the complexities in the model and present the simulation results and performance.

This high-fidelity simulation will serve as a benchmark for reduced models applicable to the optimization of the injection molding process.

Viscous Two Layer Gravity Driven Flows

Ellermeier, Wolfgang F
TU Darmstadt

09:30

The spatio-temporal evolution of disturbances in a system of two layers of viscous immiscible Newtonian liquids of constant densities in the gravitational field is investigated. The mathematical representation leads to two coupled nonlinear diffusion equations. Steady-state, constant-volume, constant-flux, waiting time solutions and stability issues are discussed, technical and geophysical implications are indicated. Physical analogies (multi-specis thermodiffusion including chemical reactions) and generalisations of similar mathematical structure are briefly indicated.

On the kinematic transport of sectional curvatures for a moving hypersurface

Fricke, Mathis (1); Köhne, Matthias (2); Vučković, Aleksandar (1); Bothe, Dieter (1)
1: TU Darmstadt
2: HHU Düsseldorf

09:50

We study the kinematic transport of a moving hypersurface, which is transported by a consistent velocity field. In particular, we are interested in the evolution of geometric quantities like the normal field and the mean curvature. The goal is to derive a system of evolution equations for these quantities. It turns out that it is useful to first consider the evolution of the so-called sectional curvature, which is defined as the curvature of the interface in a certain direction of the tangent space. The main result of this work is an evolution equation for the sectional curvature with respect to a transported tangent vector (see [2] for the transport of tangent vectors). This evolution equation contains second derivatives of the velocity field along geodesic curves and can be solved independently if the transporting velocity field is known. In this sense, the present result extends previous results [2-4], where an evolution equation is derived directly for the mean curvature. However, these equations cannot be solved directly because the rate-of-change of the mean curvature requires the knowledge of all principal curvatures. In the present approach, the evolution of the mean curvature can be inferred from the sectional curvatures.

The derived evolution equation can be used to validate the curvature transport in numerical methods for moving interfaces. As an example, we show a validation for a simple Level Set implementation.

[1] M. Fricke, M. Köhne, D. Bothe: A kinematic evolution equation for the dynamic contact angle and some consequences. Physica D: Nonlinear Phenomena, 394:26–43, DOI: 10.1016/j.physd.2019.01.008, 2019

[2] M. Kimura. Geometry of hypersurfaces and moving hypersurfaces in R^m - for the study of moving boundary problems. In M. Benes and E. Feireisl (Editors), Jindřich Nečas Center for Mathematical Modeling, Lecture notes Volume IV, Topics in Mathematical Modeling, pages 39–93. matfyzpress, Prague, 2008.

[3] J. W. Barrett, H. Garcke, R. Nürnberg: Parametric finite element approximations of curvature-driven interface evolutions, In A. Bonito and R. H. Nochetto (Editors), Geometric Partial Differential Equations - Part I, volume 21 of Handbook of Numerical Analysis, pages 275 – 423. Elsevier, DOI: 10.1016/bs.hna.2019.05.002, 2020

[4] M. Fricke: Mathematical Modeling and Volume-of-Fluid based simulation of dynamic wetting, PhD Thesis, TU Darmstadt, DOI:10.12921/tuprints-00014274, 2021

S11.03: Viscoelastic Flows, Mixture Flows and Contact Line Dynamics

Date: March 21, 2024 14:00–16:00
Room: G22/216
Chair(s): Fricke, Mathis
Maric, Tomislav

Parametric finite element approximation of two-phase Navier–Stokes flow with viscoelasticity

Garcke, Harald (1); Nürnberg, Robert (2); Trautwein, Dennis (1) 14:00
1: University of Regensburg
2: University of Trento

In this talk, we present a parametric finite element approximation of two-phase Navier–Stokes flow with viscoelasticity. The free boundary problem is given by the viscoelastic Navier–Stokes equations in the two phases, which are connected with jump conditions across the interface. The elasticity in the fluids is described with the Oldroyd-B model for the left Cauchy–Green tensor associated with the elastic part of the total mechanical response of the material, where we allow possible stress diffusion. The model was originally introduced to approximate fluid–structure interaction problems between an incompressible Newtonian fluid and a hyperelastic neo-Hookean solid, which are possible limit cases of the model.

We approximate a variational formulation for the mean curvature of the interface and for the interface evolution with a parametric finite element method. The two-phase Navier–Stokes–Oldroyd-B system in the bulk regions is discretized in a way that unconditional solvability and stability for the coupled bulk–interface system is guaranteed. Moreover, we show that the discrete Cauchy–Green tensor is positive definite. Good volume conservation properties for the two phases are observed in the case where the pressure approximation space is enriched with the help of an XFEM function. In the end, we show the applicability of our method with numerical results.

An unstructured geometrical unsplit VOF method for viscoelastic two-phase flows

Niethammer, Matthias; Asghar, Muhammad Hassan; Maric, Tomislav; Bothe, Dieter 14:40
TU Darmstadt

This study presents an unstructured geometrical Volume-of-Fluid (VOF) method [1] for two-phase flows extended with rheological constitutive models to simulate the viscoelastic behavior of liquids. A single-field formulation that results from conditional volume averaging of the local instantaneous bulk equations and interface jump conditions is employed. The method builds on the 'plicRDF-isoAdvector' geometrical VOF solver [2] that is extended and integrated with the modular framework 'DeboRheo' [3,4] for viscoelastic CFD. Utilizing a piecewise-linear geometrical interface reconstruction technique on unstructured meshes ensures numerically consistent and highly accurate discretization of viscoelastic stresses across fluid interfaces. To address challenges posed by high Deborah numbers, a stabilization approach to the constitutive equation is employed to enhance method robustness at higher fluid elasticity. The 'DeboRheo' framework [4] enables flexible combinations of different rheological models, such as Oldroyd-B, Giesekus, and many more, along with appropriate stabilization methods to address the high Deborah number problem. The theoretical formulation, implementation details, and numerical examples demonstrating the method's effectiveness in capturing viscoelastic fluid behavior are discussed. The verification study uses a droplet shear test case for a range of parameters, including Capillary number (Ca) values of 0.24, 0.4, and 0.6, as well as Deborah number (De) values ranging from De=0 to De=16. The comparative analysis of the results demonstrates the method's ability to accurately capture the behavior of viscoelastic fluids in various applications. The proposed method holds promise for enhancing the understanding and predictive capabilities of viscoelastic flows in diverse industrial and natural processes.

References
[1] Maric, T., Kothe, D.B., and Bothe, D., "Unstructured un-split geometrical volume-of-fluid methods–a review." Journal of Computational Physics 420 (2020): 109695.
[2] Scheufler, H., and Roenby, J., "Accurate and efficient surface reconstruction from volume fraction data on general meshes." Journal of computational physics 383 (2019): 1-23.
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Phase-field modeling and computation of mixture flows

ten Eikelder, Marco (1); van der Zee, Kristoffer (2); Schillinger, Dominik (1)
1: TU Darmstadt
2: University of Nottingham, UK

15:00

Many diffuse-interface Navier-Stokes Cahn-Hilliard (NSCH) models with non-matching densities have been proposed over the last decades, see e.g. [1, 2]. Even though these models aim to represent the same physical phenomena, they seem to differ at first sight. The first objective of this talk is to present a framework for NSCH models that unites all of these models [3]. Our development is based on three unifying principles: (1) there is only one system of balance laws based on continuum mixture theory that describes the physical model, (2) there is only one natural energy-dissipation law that leads to quasi-incompressible NSCH models, (3) variations between the models only appear in the constitutive choices. At this point, our framework for NSCH models with non-matching densities is not fully compatible with mixture theory. Namely, it represents reduced models in which the evolution equations for the diffusive fluxes are replaced by constitutive models. The second objective of this talk is to present a new incompressible model that guarantees full compatibility with mixture theory by replacing the energy-dissipation law by the second law of thermodynamics [4]. We compare this model, analytically and computationally, to existing NSCH models with non-matching densities. We conclude the talk by discussing a divergence-conforming isogeometric finite element discretization, and showing relevant benchmark computations such as a rising air bubble in water and the contraction of a liquid filament [5].

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[3] 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 33 (2023), 175-221.

[4] ten Eikelder, M.F.P., van der Zee, K.G., and Schillinger, D., Thermodynamically consistent diffuse-interface mixture models of incompressible multicomponent fluids. arXiv preprint arXiv:2302.09287.

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Bridging the scales in capillary rise dynamics with complexity-reduced models

Fricke, Mathis (1); Raju, Suraj (1); Ouro-Koura, El Assad (1); Kozymka, Olena (1); De Coninck, Joel (2); Tukovic, Zeljko (3); Maric, Tomislav (1); Bothe, Dieter (1)

1: TU Darmstadt
2: Université libre de Bruxelles, Belgium
3: University of Zagreb, Croatia

15:20

Dynamic wetting processes inherently manifest as multiscale phenomena. While the capillary length is typically millimeters, solid-liquid interactions occur at the nanometer scale. These short-range interactions significantly affect macroscopic behaviors like droplet spreading and menisci dynamics. The Navier slip length, determined by liquid viscosity and solid-liquid friction, plays a crucial role in three-phase contact line dynamics. It varies from nanometers (hydrophilic surface) to microns (hydrophobic surface). However, resolving it in computational fluid dynamics (CFD) simulations can be computationally expensive. In this study, we propose simplified ordinary differential equation (ODE) models, leveraging local dissipation rates from Stokes flow solutions near the moving contact line, to bridge the nanoscale physics and macroscopic dynamics. Our ODE model accurately predicts the impact of the slip parameter in fully resolved CFD simulations, focusing on capillary rise dynamics.

[1] M. Fricke, S. Raju, E. A. Ouro-Koura, O. Kozymka, J. De Coninck, Z. Tukovic, T. Maric, D. Bothe: Bridging the scales in capillary rise dynamics with complexity-reduced models, Preprint, https://doi.org/10.48550/arXiv.2311.11947, 2023

S12: Waves and Acoustics

Organizer(s): Rauter, Natalie *(Helmut-Schmidt-University / University of the Federal Armed Forces Hamburg)*
Weber, Wolfgang *(Helmut Schmidt University / University of the Federal Armed Forces Hamburg)*

S12.01: Waves and Acoustics

Date: March 20, 2024 14:00–16:00
Room: G22/112
Chair(s): Rauter, Natalie
Weber, Wolfgang

Integrated approach for automated structural health monitoring of steel pipes through long-range ultrasonic testing and machine learning

Kapoor, Garima (1); Boll, Benjamin (1); Wasif, Rukhshinda (2); García, Amaya (3); Pinson, Ivan (2); Abarkane, Chihab (3); Akram, Shahbaz (2); Hoeche, Daniel (1); Feiler, Christian (1); Zheludkevich, Mikhail (1)

1: Helmholtz-Zentrum Hereon
2: Innerspec Technologies, UK
3: CIDETEC, Spain

14:00

Corrosion Under Insulation (CUI) poses significant risks to the structural integrity of thermally insulated equipments in the onshore and offshore oil and gas industries. This research contributes towards the development of automated pipeline condition monitoring system. It involves the detection and severity assessment of corrosion damage in steel pipes through the integration of Machine Learning (ML) and Non-Destructive Testing (NDT) using Finite Element Analysis (FEA) and experimental data.

Utilizing the COMSOL Multiphysics platform, defects of varying characteristics (including size, shape, corrosion products) were simulated to mimic the corrosion-induced anomalies. The Long-Range Ultrasonic Testing (LRUT) model was developed to capture the ultrasonic wave interactions with these defects, generating a comprehensive dataset. Furthermore, the signal processing techniques such as wavelet transform were applied to enhance the interpretability of the acquired signals. The transformed signals subsequently served as input to ML models, establishing a correlation between signal characteristics and corrosion severity levels (low, medium, high). The performance of different ML models was compared. This integrated approach aims to provide a reliable and automated system for real-time structural health monitoring of steel pipes. The proposed methodology offers a promising solution for early and accurate identification, as well as severity classification of corrosion damage, thereby facilitating proactive maintenance strategies in critical infrastructural applications.

Optimizing Structural Health Monitoring Systems: A 2D Numerical Investigation on Impedance Matching for FML with Integrated Sensors

Rottmann, Max; Mangalath, Clara; Weber, Wolfgang E.

Helmut Schmidt University, University of the Federal Armed Forces Hamburg

14:20

Fibre Metal Laminates (FML) represent an innovative class of advanced composite materials that integrate the mechanical properties of both metals and fibre-reinforced composites (FRP). Combining the strength and ductility of metals with the lightweight and high stiffness of FRP, FMLs have emerged as new material combinations for applications in aerospace, automotive, and other engineering disciplines. Structural health monitoring (SHM) using guided ultrasonic waves (GUW) is the state-of-the-art for non-destructive testing of thin-walled structures. When applied to FML, SHM plays a crucial role in monitoring the integrity over time and detecting potential damage such as delamination, fibre breakage or other structural anomalies. In SHM with GUW a wave-field is emitted by actuators. This wave-field can be affected by damage in the structure, thereby changing its propagation characteristics. Sensors monitor the interaction between damage and GUW, which can be utilized to locate the damage and evaluate the health state of the structure.

In this study, a key aspect of SHM for FML includes the integration of e.g. sensors and actuators within the laminate structure to monitor damage in the FRP layers. Sensor integration into FML allows for improved monitoring capabilities in comparison to measuring techniques like laser vibrometers, which are limited to measuring displacements on the exterior of the structure. However, the integration of sensors and actuators yields the technical difficulty of distorting the wave fields and may result in an over- or underestimation of damage. Similar to damage, the distortion of the wave-field is caused by the changes in acoustic impedance resulting from different material properties. In the previous study [1], incorporating a functionally graded artificial interphase through acoustic impedance matching between the sensor and host material showed significant outcomes. The current contribution extends the prior interphase for an isotropic homogeneous material to a FML structure.

This paper presents a numerical simulation study on a two-dimensional model of FML with integrated sensors. The interphases are designed based on impedance matching, which improves signal transmission and reduces disturbing reflections. The conducted investigations hold for several interphase configurations for a wide frequency range. The optimized integration of sensors demonstrates promising results for enhancing the reliability and accuracy of SHM systems. This research serves as a foundation for further experimental validation and the development of advanced sensor-integrated FML structures with improved monitoring capabilities.

[1] Rottmann, M. et al.: A numerical study on planar gradient acoustic impedance matching for guided ultrasonic wave detection. DOI: 10.1177/10775463221149764.

Analysis of wave scattering at the common interface of piezoelectric media half-spaces under surface/interface elasticity theory

Nath, Arindam; Dhua, Sudarshan 14:40
National Institute of Technology Andhra Pradesh, India

The study investigates the reflection and refraction phenomena of shear horizontal waves at the interface between two piezoelectric media in the scope of surface/interface elasticity. In micro/nano smart structures such as Surface Acoustic Wave devices, where the ratio of the area of the surface/interface to the bulk is large, the produced field quantities are affected by surface/interface electromechanical properties. The Gurtin-Murdoch (1975) and Eremeyev (2016) approaches have been used to derive the surface strain energy density, surface stress tensor, and surface kinetic energy density, accounting for the surface/interface energy. The expressions of the amplitudes of reflected and refracted waves have been derived analytically using the governing equations of a piezoelectric medium. Numerical simulations and graphical interpretations have been carried out to observe the effects of surface/interface elasticity on wave propagation. It has been found that the wave's amplitude ratios are sensitive to changes in surface/interface elasticity parameters. The investigation may have possible applications in signal processing, transduction, and frequency shifting (a difference in the velocity of surface waves and controlling the selectivity of a filter compensation) of individual devices.

Surface effects on wave propagation in piezoelectric-piezomagnetic bilayer loosely bonded thin plates using nonlocal theory of elasticity

Mondal, Subrata; Dhua, Sudarshan 15:00
National Institute of Technology Andhra Pradesh, India

This study explores the dispersion characteristics of Shear Horizontal (SH) waves in imperfectly bonded piezoelectric (PE) and piezomagnetic (PM) bilayer plates, considering nonlocal and surface effects. Utilizing the nonlocal Magnetoelectroelastic (MEE) theory with inherent length, governing equations are derived. The G-M model and generalized Young-Laplace equations are employed to incorporate surface effects into the boundary conditions. Analytical solutions yield a closed-form dispersion equation for electrically open and magnetically short conditions. Numerical analysis reveals the significant influence of nonlocal scale parameters and surface parameters on SH surface wave propagation. Contrary to classical theory, the study emphasizes the heightened impact of coupling nonlocal small-scale and surface piezoelectricity effects. Notably, imperfectness across the interface and bilayer thickness ratio exhibit substantial effects on phase velocity. 2D and 3D mode shapes plots

for SH wave propagation are provided. This research offers valuable insights into complex wave dynamics, contributing to the optimization of smart composites for enhanced performance in diverse engineering applications.

S12.02: Waves and Acoustics

Date: March 20, 2024 16:30–18:30
Room: G22/112
Chair(s): Weber, Wolfgang
Rauter, Natalie

An investigation of wave characteristics in Peridynamic media using Nonlocal Helmholz decomposition

Dhua, Sudarshan; Mondal, Subrata
National Institute of Technology Andhra Pradesh, India
16:30

The study explores Peridynamics (PD), a theoretical framework utilizing integro-differential equations, an alternative to classical partial differential equations in continuum mechanics. Employing non-local Helmholtz-Hodge decomposition in isotropic peridynamic media, the research presents a novel method to decompose the displacement field into divergence-free and curl-free components. Investigating planar harmonic wave propagation in nonlocal elastic solid mediums, the study derives dispersion relations for longitudinal and transverse waves. Using Green's function technique, the closed-form of general solutions for initial-value problems are derived. Examining exponential, Gaussian, and constant kernels, the research utilizes numerical solutions to demonstrate phase velocity and group velocity variations with respect to alterations in the non-local length parameter. The findings not only theoretical understanding but also have practical implications for optimizing the dynamic performance of mechanics and materials in engineering and related disciplines.

Impact of Surface/interface effect on the propagation of shear wave in a composite piezoelectric cylinder

Maji, Arpita; Dhua, Sudarshan
National Institute of Technology Andhra Pradesh, India
16:50

The investigation of the surface/interface effect on the propagation behavior of shear acoustic wave in a thin, layered piezoelectric cylinder. The effects of surface and interface in the boundary of piezoelectric material are considered. The dispersion relation under electrically short and open conditions has been determined analytically using a special function. Dispersion curves have been plotted to illustrate the salient features of parameters like surface piezoelectric parameter, surface elasticity parameter, surface density, and radius ratio of a concentric cylinder using numerical simulation. It has been found that the size-dependent parameters have an effective difference only when the thin piezoelectric layer is considered.

A case study on the damage detection of beams via the time reversal method

Huguet, Mélissandre; Ture Savadkoohi, Alireza; Lamarque, Claude-Henri
Université de Lyon, ENTPE, École Centrale de Lyon, CNRS, LTDS, UMR5513, France
17:10

The domain of structural health monitoring (SHM) aims to control the integrity and performance of different types of structural systems such as bridges, and their components, e.g. cables through the use of sensors, monitoring systems and analysis tools. To this end, non-destructive testing (NDT) techniques are developed in order to detect and to identify anomalies such as cracks, while guaranteeing the safety and durability of structural systems, their components and their users. The SHM houses many techniques covering from static/quasi-static to dynamic based methods via exploiting the collected data ranged from mechanical vibration fields to acoustic and ultrasonic domains.

Nowadays, the ultrasonic techniques are used more often in NDT due to their easy implementation and their capabilities in the detection of flaws at their early developments. Meanwhile, in the classical use the operator needs a prior knowledge on the structure under investigation in order to establish a

correspondence between the information obtained during the ultrasonic test and the state of health of the system.

This study focuses on ultrasonic techniques and in particular on the use of time reversal (TR) method. The TR is based on the time symmetry nature of solutions of the wave equation in an undamaged medium. The TR method benefits from its self-adaptive focalization capability, without a prior knowledge of the system, leading to detection of flaws, even at their early stages of developments.

This study presents the damage detection of a set of metallic beams with different types of damage indices via classical ultrasonic method and then by the TR technique. A multi-phased array probe is endowed at high frequencies with, for classical method, the study of the beam's characteristics such as velocity of waves. Then, TR technique is exploited to detect, to locate and to quantify damages on studied beams. Finally, the TR method is applied to finite element models of the considered beams and results are compared with those obtained from experimental works.

S13: Flow control

Organizer(s): Peitz, Sebastian *(Paderborn University)*
Semaan, Richard *(Technische Universität Braunschweig)*

S13.01: Flow control (vehicles and drag reduction)

Date: March 19, 2024 16:30–18:30
Room: G22/216
Chair(s): Heiland, Jan
Peitz, Sebastian

Active flow control for road vehicles

Krajnovic, Sinisa 16:30
Chalmers University of Technology, Sweden

Development of active flow control for improvement of aerodynamic performance of road vehicles will be discussed. We will start with the motivation and the fundamentals of the active flow control and show how the active flow control can be used for different vehicle applications. The usage of both numerical and experimental techniques will be demonstrated, and we will show how these should be used for optimal results of the flow control. The complete process of the flow control development for a vehicle, from fundamental studies to application on the full-scale vehicle, will be presented.

Modeling for surrogate-based optimization of actuation parameters for active drag reduction in turbulent boundary layer flows

Hübenthal, Fabian; Meinke, Matthias; Schröder, Wolfgang 17:10
RWTH Aachen University

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, aerodynamic improvements are needed to reduce energy demand and costs.
A promising technique to actively reduce the aerodynamic viscous drag are spanwise traveling transversal surface waves to manipulate the near-wall turbulent boundary layer, which is less well studied than passive techniques such as riblet surfaces. From an optimization perspective, given the flow conditions, e.g., specified by the Reynolds and Mach numbers, the goal is to choose the actuation parameters, i.e., amplitude, wavelength, and period, such that the drag reduction and the net power savings are optimized, while other aerodynamic properties, such as the lift-to-drag ratio for airfoils, are neutrally or positively affected.
The partially conflicting objectives, i.e., drag reduction and net power savings, are evaluated using wall-resolved large-eddy simulations (LESs) based on the body-fitted deformable structured grid finite volume solver part of the in-house solver framework m-AIA. Since wall-resolved LESs of turbulent boundary layer flows are computationally expensive and the design space of choices is too vast to be sufficiently investigated by grid search methods, surrogate-based optimization is selected to guide the determination of optimal actuation settings.
To succeed, the non-sequential original problem is reformulated into an iterative auxiliary problem for sequential surrogate-based optimization by addressing the trade-off between exploration and exploitation using the concept of Bayesian optimization. The primary goal is to reduce the number of resource-intensive large-eddy simulations while still achieving a satisfactory optimum, insightful data, and interpretative knowledge.
For this reason, surrogate modeling includes not only the interpolation of sequentially updated simulation-based data points, but also the integration of prior knowledge to enhance the quality of inter- and extrapolation, as well as the iterative updating of the feasible set of the optimization. In this study, support vector regression (SVR) and Gaussian process regression (GPR) based models are analyzed and compared in terms of the effectiveness in incorporating prior knowledge and in transferring

insights from one prior-dense objective, i.e., drag reduction, to the other prior-sparse objective, i.e., net power savings, and in terms of prediction quality to efficiently guide the surrogate-based optimization loop.

Numerical investigation of drag reduction effects on a track bicycle fork using airfoils with a wavy leading edge

Klein, Marten (1,2); Kessler, Robert William (1); Schmidt, Heiko (1,2)
1: BTU Cottbus-Senftenberg
2: Scientific Computing Lab, Energy Innovation Centre, Cottbus

17:30

Airfoils are frequently used to reduce the aerodynamic drag of bluff bodies, which has been recognized also in cycling. Here, the focus is on the fork of a track bike, for which it has been hypothesized that additional drag reduction is possible by a passive flow control mechanism utilizing a wavy leading edge (WLE). The WLE geometry is inspired by whale fins. Due to the historic interest in aviation, the lift-to-drag ratio of WLE airfoils has been investigated previously, but no study so far has addressed the aerodynamic drag at moderately high Reynolds numbers for zero-lift configurations.

The WLE configuration investigated here is based on a symmetric straight leading edge (SLE) profile. This SLE profile has a thickness of d = 11 mm and a chord length of c = 80 mm, motivated by the current regulations of the Union Cycliste Internationale (UCI). The WLE airfoil is parameterized by circular arc segments with cross-stream wavelength w, amplitude a, and edge radius k. The angle of attack is 0°. The Reynolds number is Re = 88,000 based on the target velocity, the chord length of the SLE base profile, and the density and viscosity of air at standard conditions. Wall-resolved Reynolds-averaged Navier–Stokes simulations (RANS) are performed for 50 geometries. Selected cases are complemented by large-eddy simulations (LES). Both approaches are used to compute the aerodynamic drag coefficient C_d in order to compensate for the variation in the frontal area of the WLE and SLE airfoils investigated. Present RANS and LES predict that C_d reduces with increasing wave amplitude a, but only up to a/c = 0.2 for the selected geometry. The drag reduction effect is almost independent of the wavelength w once the ratio c/w is large enough. This suggests that the ratio of wave amplitude and thickness, a/d, is the limiting geometry parameter. Preliminary LES suggest that the WLE induces counter-rotating vortex pairs, modifying the turbulent flow structures in the wake, the vortex shedding, and some upstream properties of the external flow. Correspondingly, the pressure drag and viscous drag contributions vary with the geometry.

In the talk, the focus is on the RANS results, but LES will be discussed in addition. Aspects of aerodynamic drag and wake properties due to airfoil shape modifications are addressed specifically from the perspective of high-performance track cycling.

S13.02: Flow control (turbulence and reduced-order modelling)

Date: March 22, 2024 08:30–10:30
Room: G22/216
Chair(s): Peitz, Sebastian
Heiland, Jan

Reduced Order Modelling in Fluid Mechanics: focus turbulence and compressibility

Rozza, Gianluigi
International School for Advanced Studies, Italy

08:30

We do provide the state of the art of Reduced Order Methods (ROM) for parametric Partial Differential Equations (PDEs), and we focus on some perspectives in their current trends and developments, with a special interest in parametric problems arising in offline-online Computational Fluid Dynamics (CFD).

Recent developments involve a better integration of emerging topics with model reduction, such as high performance computing (HPC), uncertainty quantification (UQ), data science (DS), machine learning (ML) in a data driven perspective, in order to allow a better exploitation of digital twins.

All the previous aspects are quite relevant – and often challenging — when well integrated also in CFD problems, including turbulence, to focus on real time simulations for complex parametric industrial, environmental and biomedical flows, or even in a flow control/inverse problems setting with data assimilation.

Crucial aspects to be addressed are related with uniqueness, stability, accuracy, as well as reliability of solutions. Some model problems will be illustrated by focusing on few benchmark study cases, for example on fluid-structure interaction problems and/or on shape optimisation, applied to some industrial and applied science problems of interest.

Model-based deep reinforcement learning for flow control

Weiner, Andre (1); Geise, Janis (2)
1: TU Dresden
2: TU Braunschweig

09:10

Deep reinforcement learning (DRL) algorithms had their first big breakthrough in the field of computer gaming but in recent years, the same algorithms have also become popular in the fluid mechanics community, for example, to solve flow control problems or to improve turbulence modeling. One example demonstrating the huge potential and flexibility of DRL is its recent application to algorithmic discovery.
In the field of fluid mechanics, DRL has been combined mostly with computational fluid dynamics (CFD). However, due to the necessity of repeatedly running time-resolved simulations, only relatively simple test cases that can be solved in a matter of minutes or a few hours have been considered so far. On the path to applying DRL to more complex scenarios, the sample efficiency of available algorithms has to be improved.
One approach to deal with computationally expensive environments is model-based DRL, where the environment/simulation is partially replaced with an additional model. However, model bias can quickly lead to a failure of policy optimization. One way to deal with model uncertainty is learning from model ensembles. In our contribution, we discuss potential modeling approaches for CFD environments and show results for vanilla and ensemble model-based DRL. We believe that model-based DRL will be a crucial enabler for the success of DRL applied to technically relevant applications of flow control or turbulence modeling.

A volume-averaging and stochastic turbulence modeling framework for homogeneous roughness-induced drag in turbulent flows

Medina Méndez, Juan A. (1); Parra Lafuente, Adrián (2); Schmidt, Heiko (1)
1: BTU Cottbus-Senftenberg
2: Polytechnic University of Madrid

09:30

The goal of this work is the formulation of a model for roughness-induced drag which can be useful for flow control applications. Recent developments on the characterization of homogeneous roughness stress the importance of two features for the evaluation of roughness-induced drag. The first one is the statistical distribution of roughness peak heights (RPH), i.e., the probability density function (PDF) of RPH. The second one is the spatial correlation of the roughness, represented by a power spectrum (PS) [1]. For PDFs or PS resembling power law behavior, the roughness characterization is similar to that of a fractal surface, for which the fractal dimension can be estimated if a given shape is assumed for distributed roughness elements, see [2, 3]. In the present work, we model rough surfaces using a fractal characterization. Subsequently, using Volume-Averaging Theory (VAT), a surface average is performed with the purpose of reducing the Navier-Stokes equations to 1-D. An effective permeability tensor is retained in this way, which can be decomposed onto a linear permeability tensor, and a dispersive nonlinear tensor. For the former, well-developed models exist, e.g., in the Darcy, or Darcy-Forchheimer regimes. For the latter, assuming that Reynolds numbers are sufficiently large as to anticipate an effect of the turbulent flow, we choose a modeling strategy based on a stochastic turbulence model. The choice is unique in the sense that it reproduces 3-D turbulence dynamics in 1-D domains, One-Dimensional Turbulence (ODT) [4]. Simulations are carried out in order to evaluate the effects of different types of roughness on turbulent channel flows. In order to verify the

model performance, results are compared to existing Direct Numerical Simulation data available on skin friction drag, mean velocity profiles, and other wall-normal profiles of stress contributions [5]. Overall, reasonable agreement is obtained. Thus, by using the suggested model, it is possible to derive the features of rough surfaces which can achieve a desired drag modification in turbulent flow applications.

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Multi-fidelity surrogate modeling of the response of an actuated turbulent boundary layer

Olivucci, Paolo (1); Semaan, Richard (1); Albers, Marian (2); Shao, Xiao (2); Schroeder, Wolfgang (2) 09:50
1: TU Braunschweig
2: RWTH Aachen University

Active wall motion control for frictional drag reduction in turbulent boundary layers includes a number of techniques, such as spanwise wall oscillation, traveling waves of spanwise velocity, traveling wall-normal deflection, and others. In this study, we consider the response of periodic, wall-normal displacement of the wall surface that travels in the spanwise direction, which is a proven wall control actuation technique.

The net power saving (NPS) is a key metric used to evaluate the actuation efficiency. A multi-fidelity surrogate model of the NPS response to a range of actuation settings is constructed using a Gaussian Process (GP) framework. The modeling approach relies on two multi-fidelity data sets. The predictive performance of the model is shown to be superior to the single-fidelity model, as evidenced by higher cross-validated accuracy scores, including mean log-likelihood values. The model is used to infer a detailed dependence of the flow response on the control parameters, the existence of maxima, and their physical underpinnings.

Distributed control of Rayleigh–Bénard convection using symmetry-exploiting deep reinforcement learning

Chidananda, Vikas; Peitz, Sebastian 10:10
Paderborn University

We present a convolutional framework which significantly reduces the complexity and thus, the computational effort for distributed reinforcement learning control of dynamical systems governed by partial differential equations (PDEs). Exploiting translational equivariances, the high-dimensional distributed control problem can be transformed into a multi-agent control problem with many identical, uncoupled agents. Furthermore, using the fact that information is transported with finite velocity in many cases, the dimension of the agents' environment can be drastically reduced using a convolution operation over the state space of the PDE, by which we effectively tackle the curse of dimensionality otherwise present in deep reinforcement learning. In this setting, the complexity can be flexibly adjusted via the kernel width or by using a stride greater than one (meaning that we do not place an actuator at each sensor location). Moreover, scaling from smaller to larger domains – or the transfer between different domains – becomes a straightforward task requiring little effort. We use our framework to study a particularly challenging and relevant PDE system, namely Rayleigh–Bénard convection. Employing low-dimensional proximal policy optimisation (PPO) agents, we effectively reduce the Nusselt number of the system, which is a measure of convective heat transfer. Furthermore, we

show the agents trained in such a paradigm generalizes well not only to longer time horizons, but also to increasingly chaotic flow regimes characterised by Rayleigh number (Ra) with little or no retraining.

S14: Applied analysis

Organizer(s): Liao, Xian *(Karlsruhe Institute of Technology (KIT))*
Knopf, Patrik *(Universiät Regensburg)*

S14.01: Various topics in Applied analysis

Date: March 19, 2024 08:30–10:30
Room: G22/218
Chair(s): Knopf, Patrik

A degenerate cross-diffusion system as the inviscid limit of a nonlocal tissue growth model

Schmidtchen, Markus (1); Debiec, Tomasz (2); David, Noemi (3); Mandal, Mainak (1)
1: TU Dresden
2: University of Warsaw, Poland
3: University of Lyon, France

08:30

In recent years, there has been a spike in the interest in multi-phase tissue growth models. Depending on the type of tissue, the velocity is linked to the pressure through Stoke's law, Brinkman's law or Darcy's law. While each of these velocity-pressure relations has been studied in the literature, little emphasis has been placed on the fine relationship between them. In this paper, we want to address this dearth in the literature, providing a rigorous argument that bridges the gap between a viscoelastic tumour model (of Brinkman type) and an inviscid tumour model (of Darcy type).

Fast-slow limits for gradient flows on metric graphs

Heinze, Georg (1); Pietschmann, Jan-Frederik (2); Schlichting, André (3)
1: Weierstrass Institute for Applied Analysis and Stochastics
2: University of Augsburg
3: University of Münster

09:10

In this presentation, I will introduce a gradient flow model for systems of advection-diffusion equations on metric graphs. These edge-based equations are coupled by Kirchhoff conditions with additional mass reservoirs at the vertices. The resulting dynamics are described in a framework based on the Energy-Dissipation-Principle (EDP) formulation of gradient flows, allowing for the distinction between energetic and dissipative contributions to the dynamics. Building on this distinction, we explore various mechanisms leading to an acceleration of the edge dynamics while maintaining a fixed time scale for the vertex dynamics. Employing the concept of EDP convergence, this yields specific limiting dynamics defined on a (non-metric) graph. The topology of this limiting graph is determined not only by the prelimit metric graph's topology but also by the mechanism inducing the acceleration. To complement our analytical considerations, we conduct a numerical investigation into the behavior of the limiting process.

Degenerate flow and transport problems in porous media with vanishing porosity

Schulz, Raphael
Katholische Universität Eichstätt-Ingolstadt (KU)

09:30

Structural changes of the pore space and clogging phenomena are inherent to many porous media applications. However, related analytical investigations remain challenging due to potentially vanishing coefficients in the respective systems of partial differential equations. In this talk, we consider fluid flow and transport of a reactive substance in a stationary porous medium including variable porosity. We are particularly interested in analysing the model when the equations degenerate due to clogged pores, which is described by a given porosity function leading to degenerate hydrodynamic parameters. Introducing an appropriate porosity-weighted function space, we are able to handle the degeneracy and obtain analytical results. For this purpose, compactness arguments adapted to the weighted function spaces are useful. Also the decay behaviour of the solution to the transport equation with respect to the porosity is investigated. Finally, we obtain nonnegativity and boundedness for the weak solution.

Hypocoercivity in Hilbert spaces
Achleitner, Franz (1); Arnold, Anton (1); Nigsch, Eduard (1); Mehrmann, Volker (2)
1: TU Wien
2: TU Berlin
09:50

In the context of hypocoercivity for linear evolution equations with dissipation we extend equivalent characterizations that were developed for the finite-dimensional case to separable Hilbert spaces. Using the concept of a hypocoercivity index, quantitative estimates on the short-time and long-time decay behavior of a hypocoercive system are derived. The results are applied to the Lorentz kinetic equation.

Compactness and existence theory for the nonlocal radiative-temperature equation
Dematte, Elena (1); Jang, Jin Woo (2); Velázquez, Juan (1)
1: University of Bonn
2: Pohang University of Science and Technology, South Korea
10:10

We study the situation in which the distribution of temperature of a body is due to its interaction with radiation. We consider the boundary value problem for the stationary radiative transfer equation under the assumption of the local thermodynamic equilibrium and when the absorption and scattering coefficients depend on the temperature. This assumptions lead to a nonlocal nonlinear integral equation for the density of radiative energy u, which is proportional to the fourth power of the temperature due to the Stefan-Boltzmann law. In order to show existence of solutions we develop a compactness result for operators involving integrals along lines based on the study of defect measures.
This is joint work with Jin Woo Jang and Juan J. L. Velázquez

S14.02: Calculus of variations and elasticity
Date: March 19, 2024 16:30–18:30
Room: G22/218
Chair(s): Weber, Jörg

A note on the generalized Jacobian in the sense of Clarke for the inverse of a bi-Lipschitz map and applications in relaxation theory
Dolzmann, Georg; Behr, Florian
University of Regensburg
16:30

A concise summary of strategies for the analytical calculation of relaxed energies will be presented. Interesting connections with Clarke's subdifferential calculus will be indicated.

Stress-mediated growth determines E. Coli division site morphology
Allolio, Christoph (1); Chao, Luke (2,3); Dostalík, Mark (1); Pelech, Petr (1)
1: Charles University, Czech Republic
2: Harvard Medical School, USA
3: Massachusetts General Hospital, USA
16:50

Bacteria are enveloped by a rigid cell wall and replicate by cell division. During division, the cell wall needs to be drastically reshaped. It is hypothesized that the remodeling process is stress-mediated and driven by the constrictive force of a protein assembly, the Z-ring. We found that a simple large-strain morpho-elastic model can reproduce the experimentally observed shape of the division site during the constriction and septation phases of E. Coli. Our model encapsulates the multiple enzyme-dependent wall restructuring processes into a single rate. Depending on this parameter, different experimentally known morphologies can be recovered, corresponding either to mutated or wild type cells. In addition, a plausible range for the cell stiffness and turgor pressure was determined by comparing numerical simulations with experimental data on cell lysis and reported cell sacculus deformation experiments.

Navarro, P.P., Vettiger, A., Ananda, V.Y. et al. Cell wall synthesis and remodeling dynamics determine division site architecture and cell shape in Escherichia coli.

Convergence of equilibria of thin elastic plates in a discrete model - The von Kármán case
Buchberger, David; Schmidt, Bernd
University of Augsburg
17:10

In this talk we focus on the mathematical rigorous derivation of von-Karman (vK) plate theory from an atomistic model. We focus on the convergence of stationary, possibly non-minimizing points of atomistic energy functionals to the vK-functional. We distinguish between thin films and ultrathin films consisting only of a few layers. In this sense we are able to extend a recent Gamma-convergence result of Braun and Schmidt under additional assumptions on the derivative of the interaction potential. This talk is based on joint work with Bernd Schmidt.

Dimension reduction for elastoplastic rods in the bending regime
Richter, Kai; Neukamm, Stefan
TU Dresden
17:30

In our work we rigorously derive a limiting model for thin rods, starting from a full 3D model for finite plasticity. We are interested in a scaling of the elastic and plastic energy contributions like h^{-4}, where h denotes the thickness of the rod. In the limit this results in a 1D bending theory.
For the derivation we lean on the framework of evolutionary Gamma-convergence for rate-independent systems, introduced by Mielke, Roubíček and Stefanelli in 2008. The main difficulty here is to establish a mutual recovery sequence for the stored energy and dissipation. Strategies have been developed by various authors in order to construct such a sequence, e.g. for linearization or in the von Kármán regime. However, these rely on considering infinitesimal strains in the limit, which we cannot expect in the bending regime. Our approach relies on a construction based on a multiplicative decomposition of the rotation fields obtained via the rigidity estimate from Friesecke, James and Müller. In order to achieve enough regularity, we consider strain gradient terms in the energy, which act on the two parts of the polar decomposition individually. These terms vanish in the limit.

Inertial evolution of non-linear viscoelastic solids in the face of (self-)collision
Češík, Antonín (1); Gravina, Giovanni (2); Kampschulte, Malte (1)
1: Charles University, Czech Republic
2: Arizona State University
17:50

We study the time evolution of non-linear viscoelastic solids in the presence of inertia and (self-)contact. For this problem we prove the existence of weak solutions for arbitrary times and initial data, thereby solving an open problem in the field. Our construction directly includes the physically correct, measure-valued contact forces and thus obeys conservation of momentum and an energy balance. In particular, we prove an independently useful compactness result for contact forces.

S14.03: Various topics in Applied analysis

Date: March 20, 2024 08:30–09:30
Room: G22/218
Chair(s): Knopf, Patrik

Approximation and existence of a viscoelastic phase-field model for tumour growth in two and three dimensions
Garcke, Harald; Trautwein, Dennis
University of Regensburg
08:30

In the presention a phase-field model for tumour growth, where a diffuse interface separates a tumour from the surrounding host tissue is introduced. In the model, we consider transport processes by an internal, non-solenoidal velocity field. We include viscoelastic effects with the help of a general Oldroyd-B type description with relaxation and possible stress generation by growth. The elastic

energy density is coupled to the phase-field variable which allows to model invasive growth towards areas with less mechanical resistance. The main analytical result is the existence of weak solutions in two and three space dimensions in the case of additional stress diffusion. The idea behind the proof is to use a numerical approximation with a fully-practical, stable and (subsequence) converging finite element scheme. The physical properties of the model are preserved with the help of a regularization technique, uniform estimates and a limit passage on the fully-discrete level. Finally, we illustrate the practicability of the discrete scheme with the help of numerical simulations in two and three dimension

Weak stabilty of the three-dimensional axisymmetric Ericksen-Leslie model
Kortum, Joshua (1); Wang, Changyou (2)
1: JMU Würzburg
2: Purdue University, USA
09:10

From a mathematical perspective, the simplified dynamic Ericksen-Leslie model captures the essential analytical difficulties of the aforementioned model. The Ericksen-Leslie model represents one (of several) ways to attempt a description of nematic liquid crystal. It contains a Navier-Stokes-like momentum equation with (in general) singular forcing orginating from a convected harmonic map heat flow.
Up to now, an existence theory of (Leray-like) weak solutions is only available in two space dimensions. In order to start pushing the boundaries of the existence theory into the three-dimensional regime, we consider the three-dimensional axisymmetric version.
We show weak compactness of energy-bounded solutions (leading to an existence theorem for this case).
Concerning the issues in three spatial dimension, the energy might concentrate along rectifiable sets of Hausdorff-dimension one. In order to deal with this issue, we use concentration-cancellation methods at the origin of the domain as well as the axial symmetry.
Away from the origin, the concentration of energy is ruled out by a blow-up argument.

S14.04: Phase-field models
Date: March 20, 2024 14:00–16:00
Room: G22/218
Chair(s): Garcke, Harald

The Anisotropic Cahn–Hilliard Equation: Regularity Theory and Strict Separation Properties
Wittmann, Julia; Garcke, Harald; Knopf, Patrik
University of Regensburg
14:00

The Cahn–Hilliard equation with anisotropic energy contributions frequently appears in many physical systems. Systematic analytical results for the case with the relevant logarithmic free energy have been missing so far. We close this gap and show existence, uniqueness, regularity, and separation properties of weak solutions to the anisotropic Cahn–Hilliard equation with logarithmic free energy. Since firstly, the equation becomes highly non-linear, and secondly, the relevant anisotropies are non-smooth, the analysis becomes quite involved. In particular, new regularity results for quasilinear elliptic equations of second order need to be shown.

Mathematical analysis of phase separation on evolving surfaces
Caetano, Diogo (2); Elliott, Charles M. (2); Grasselli, Maurizio (1); Poiatti, Andrea (1)
1: Politecnico di Milano, Italy
2: University of Warwick, UK
14:20

In this talk I would like to present some recent results about the mathematical analysis of phase-field models on evolving surfaces. In [1] we propose the study of the Cahn-Hilliard equation on an evolving two-dimensional surface, whose evolution is assumed to be given *a priori*. We prove the instantaneous regularization property of weak solutions and show the validity of the instantaneous strict separation property. Applications of these models can be found, for instance, in the cell membrane

phase separation. Nevertheless, the evolution in time of the surface should not be *a priori* prescribed. Taking inspiration from the recent [3], we derived a system of equations coupling a multi-component Cahn-Hilliard equation with a fourth order equation for the evolution of the surface, under the assumption of small deformations. The spherical surface evolves in time due to the presence of the different chemical species undergoing phase separation. We analyze this system in [2] and obtain the well-posedness of weak solutions, together with their instantaneous regularization and the validity of the instantaneous strict separation property. In conclusion, we show the convergence of each trajectory to a single equilibrium.

References

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On a convective Cahn-Hilliard system with dynamic boundary conditions

Stange, Jonas; Knopf, Patrik
University of Regensburg

14:40

We consider a general class of bulk-surface convective Cahn-Hilliard systems with dynamic boundary conditions. In contrast to classical Neumann boundary conditions, the dynamic boundary conditions of Cahn-Hilliard type allow for dynamic changes of the contact angle between the diffuse interface and the boundary, a convection-induced motion of the contact line as well as absorption of material by the boundary. The coupling conditions for bulk and surface quantities involve parameters K, L in $[0,\infty]$, whose choice declares whether these conditions are of Dirichlet, Robin or Neumann type.
In this talk, I present some recent results on the well-posedness of this system. For regular potentials, the existence of weak solutions in the case K, L in $(0,\infty)$ are proven by means of a Faedo-Galerkin approach, whereas for all other cases, the existence is shown by means of the asymptotic limits, where K and L are sent to zero or to infinity, respectively. Eventually, we establish higher regularity for the phase-fields, and we prove (weak-strong) uniqueness of weak solutions under additional assumptions on the mobility functions. Finally, we prove analogous results in the case of singular potentials. For the analysis in this case, we regularise singular potentials by a Yosida approximation, which allows us to apply the results for regular potentials, and eventually pass to the limit in this approximation scheme.
This is based on joint work with Patrik Knopf (Universität Regensburg).

Existence of weak solutions to a Cahn-Hilliard-Biot system

Abels, Helmut; Garcke, Harald; Haselböck, Jonas
University of Regensburg

15:00

We prove existence of weak solutions to a diffuse interface model describing the flow of a fluid through deformable porous media consisting of two phases. The system nonlinearly couples Biot's equations for poroelasticity, including phase-field dependent material properties, with the Cahn–Hilliard equation to model the evolution of the solid, and is further augmented by a viscoelastic regularization consistent with secondary consolidation. To obtain this result, we approximate the problem in two steps, where first a semi-Galerkin ansatz is employed to show existence of weak solutions to regularized systems, for which later on compactness arguments allow limit passage. Notably, existence of approximate solutions in the first step is reduced to a fixed-point problem and an application of maximal L^p-regularity theory in Bessel-potential spaces yields the regularity we require to pass to the limit.

Curvature-driven pattern formation in Biomembranes
Pešić, Anastasija 15:20
Humboldt-Universität zu Berlin

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 renders the resulting functionals nonlocal. In this talk, we will discuss the scaling behavior of the infimal energy in terms of the problem parameters, i.e., parameters related to surface tension, line tension, bending rigidity, and strength of the composition-curvature coupling. Additionally, some limiting models in terms of Gamma-convergence will be presented. The talk is based on a joint work with Janusz Ginster and Barbara Zwickangl.

Nonlocal-to-Local Convergence for a Diffuse Interface Model for Two Phase Flow with Matched Densities
Hurm, Christoph (1); Abels, Helmut (1); Knopf, Patrik (1); Poiatti, Andrea (2) 15:40
1: University of Regensburg
2: Politecnico di Milano, Italy

We prove convergence of a sequence of weak solutions to a diffuse interface model for the two-phase flow of incompressible fluids with matched densities with a nonlocal Cahn-Hilliard equation to the strong solution to the corresponding system with a standard local Cahn-Hilliard equation. The analysis is done in the case of periodic boundary conditions and a regular double-well potential. The proof is based on the energy method and convergence of the linearized operators in the Cahn-Hilliard equations.

S14.05: PDEs related to fluid mechanics
Date: March 20, 2024 16:30–18:30
Room: G22/218
Chair(s): Liao, Xian

Time-periodic flow past a body: Approximation by problems on bounded domains
Eiter, Thomas 16:30
University of Kassel

We consider the time-periodic flow of an incompressible viscous fluid past a body. For numerical implementations, the problem has to be reduced to a bounded domain, which is achieved by introducing an artificial boundary. To be a good approximation of the original problem, the associated boundary conditions have to reflect the asymptotic behavior of the flow in the exterior domain. This behavior is studied in terms of new representation formulas that rely on the time-periodic fundamental solutions to the linearized Navier-Stokes equations.

Rotating solutions to the incompressible Euler-Poisson equation with external particle
Alonso-Orán, Diego (2); Kepka, Bernhard (1); López-Velázquez, Juan (1) 17:10
1: University of Bonn
2: Universidad de La Laguna, Spain

We consider an incompressible, two-dimensional fluid body, together with a self-induced attractive force. Furthermore, it is perturbed by an external particle with small mass. The shape of the body is assumed to be close to the disk, changing due to the interaction with the particle. In addition, the whole configuration rotates around its center of mass.

We construct solutions to the incompressible Euler-Poisson equation, which are associated with steady states in a rotating coordinate system, via perturbative methods. Moreover, we study a large

class of internal motion of the fluid body. To this end, we apply the Grad-Shafranov method as well as conformal mappings.

Quantitative Analysis for the Ill-Posedness of the Prandtl Equations
De Anna, Francesco (1); Kortum, Joshua (1); Scrobogna, Stefano (2)
1: JMU Würzburg
2: University of Trieste
17:50

The Prandtl theory of boundary layers has significantly impacted various scientific disciplines. However, despite its widespread use, the solutions to the underlying equations exhibit inherent instability. Recent research by Gérard-Varet and Dormy showed that the equations are ill-posed in Sobolev spaces (without making structural assumptions on the flow). Around a suitable shear flow, they determined a dispersion relation on the frequencies, which was interpreted later on as ill-posedness in a more general class of functions (the so-called Gevrey-classes m, m>2). This talk intends to present a recent result, obtained in collaboration with S. Scrobogna (University of Trieste) and J. Kortum (University of Würzburg). Through a quantitative analysis of instabilities and norm inflations, we demonstrate that, mathematically, the ill-posedness is momentarily valid in Sobolev spaces, leaving the ill-posedness in Gevrey classes m>2 as still an open problem. We also explore related issues concerning the ill-posedness of a meaningful extension of the Prandtl Equations.

S14.06: Hyperbolic PDEs

Date: March 21, 2024 08:30–10:30
Room: G22/218
Chair(s): Liao, Xian

Modeling and optimization of optical resonances.
Karabash, Illia
University of Bonn
08:30

It is planned to review recent mathematical studies of resonance optimization for optical cavities and compare them with the state of art in the applied physics field of high-Q optical resonators. The main attention will be devoted to the modeling of the leakage of energy into uncertain or random surrounding environment and to analytical difficulties of the optimization for Maxwell systems. In particular models of random resonances will be discussed.

Parameter-asymptotic behavior of integro-differential models of nonlinear acoustics
Meliani, Mostafa
Radboud University, The Netherlands
09:10

In this talk, we will discuss the well-posed and asymptotic behavior of quasilinear integro-differential equations describing the evolution of ultrasound in complex media exhibiting so-called anomalous diffusion of Gurtin–Pipkin type. The analysis is carried out uniformly with respect to some small involved parameter on which the memory kernels depend and which can be physically interpreted as the sound diffusivity or the thermal relaxation time. We then analyze the behavior of solutions as this parameter vanishes, and in this way relate the equations to their limiting counterparts. Furthermore, we establish the convergence rates in appropriate norms.

The talk is based on [1, 2].

[1] Barbara Kaltenbacher, Mostafa Meliani, and Vanja Nikolić. "Limiting behavior of quasilinear wave equations with fractional-type dissipation." *arXiv preprint arXiv:2206.15245* (2022).

[2] Barbara Kaltenbacher, Mostafa Meliani, and Vanja Nikolić. "The Kuznetsov and Blackstock equations of nonlinear acoustics with nonlocal-in-time dissipation." *arXiv preprint arXiv:2308.10580* (2023).

Large Data Solutions to 1-D Hyperbolic Systems, Ill-Posedness, and Convex Integration
Krupa, Sam Gittleman; Székelyhidi, László
Max Planck Institute for Mathematics in the Sciences, Leipzig 09:30

For hyperbolic systems of conservation laws in one space dimension endowed with a single convex entropy, it is an open question if it is possible to construct solutions via convex integration. Such solutions, if they exist, would be highly non-unique and exhibit little regularity. In particular, they would not have the strong traces necessary for the nonperturbative L^2 stability theory of Vasseur. Whether convex integration is possible is a question about large data, and the global geometric structure of genuine nonlinearity for the underlying PDE. In this talk, I will discuss recent work which shows the impossibility, for a large class of 2x2 systems, of doing convex integration via the use of T_4 configurations. Our work applies to every well-known 2x2 hyperbolic system of conservation laws which verifies the Liu entropy condition. This talk is based on joint work with László Székelyhidi.

Self-similar behaviour for Boltzmann-type equations
Throm, Sebastian
Umeå University, Sweden 09:50

This talk considers self-similar behaviour for kinetic equations of Boltzmann type. More precisely, we will discuss the question of uniqueness of self-similar profiles. The approach relies on a perturbation argument from constant interaction kernels and involves a careful analysis of the corresponding linearised operator.
This includes joint work with R. Alonso, V. Bagland, J. Canizo and B. Lods

Bifurcation and Asymptotics of Cubically Nonlinear Transverse Magnetic Surface Plasmon Polaritons
He, Runan
Martin Luther University Halle-Wittenberg 10:10

Linear Maxwell equations for transverse magnetic (TM) polarized fields support single frequency surface plasmon polaritons (SPPs) localized at the interface of a metal and a dielectric. Metals are typically dispersive, i.e. the dielectric function depends on the frequency. We prove the bifurcation of localized SPPs in dispersive media in the presence of a cubic nonlinearity and provide an asymptotic expansion of the solution and the frequency. We also show that the real frequency exists in the nonlinear setting in the case of PT-symmetric materials. This talk is based on joint works with Tomas Dohnal (Halle).

S14.07: Various topics in Applied analysis
Date: March 21, 2024 14:00–16:00
Room: G22/218
Chair(s): Schmidtchen, Markus

Analysis of a drift-diffusion model for perovskite solar cells
Glitzky, Annegret
Weierstrass Institute for Applied Analysis and Stochastics 14:00

We present the analysis of an instationary drift-diffusion model for perovskite solar cells using Fermi–Dirac statistics for electrons and holes and Blakemore statistics for the mobile ions in the perovskite. The free energy functional we work with is related to this choice of the statistical relations.

To prove the existence of weak solutions, we consider a problem with regularized state equations on any arbitrarily chosen finite time interval. We ensure its solvability by time discretization and passage to the time-continuous limit. Positive lower and upper a priori estimates for the densities of its solutions that are independent of the regularization level ensure the existence of solutions to the original problem.
Furthermore, we derive for these solutions upper bounds (strictly below the density of transport states) for the ionic species. The estimates for the densities rely on Moser iteration techniques.

Analysis of a Soap Film Catenoid Driven by an Electrostatic Force

Schmitz, Lina
Leibniz University Hannover

14:40

A conductive soap film spanned between two parallel rings of equal radius takes the shape of a catenoid. Applying a voltage difference between this catenoid and an outer metal cylinder induces an electrostatic force deflecting the film. Its evolution can be modeled by a parabolic equation coupled with an elliptic equation for the electrostatic potential in the unknown domain between outer cylinder and soap film. For the rotational symmetric case, I will explain how this free boundary problem can be recast as a single parabolic equation with a non-local source term. I will also present results on existence and stability of stationary solutions.

New results on global bifurcation of travelling periodic water waves

Weber, Jörg
University of Vienna, Austria

15:00

While the research on water waves modeled by Euler's equations has a long history, mainly in the last two decades travelling periodic rotational waves have been constructed rigorously by means of bifurcation theorems. After introducing the problem, I will present a new reformulation in two dimensions in the pure-gravity case, where the problem is equivalently cast into the form "identity plus compact", which is amenable to Rabinowitz's global bifurcation theorem. The main advantages (and the novelty) of this new reformulation are that no simplifying restrictions on the geometry of the surface profile and no simplifying assumptions on the vorticity distribution (and thus no assumptions regarding the absence of stagnation points or critical layers) have to be made. Within the scope of this new formulation, global families of solutions, bifurcating from laminar flows with a flat surface, are constructed. Moreover, I will discuss the possible alternatives for the global set of solutions, as well as their nodal properties. This is joint work with Erik Wahlén.

The two-phase periodic Stokes flow in the plane driven by surface tension and gravity

Böhme, Daniel
University of Regensburg

15:20

We study the two-phase Stokes flow driven by surface tension and gravity under the assumption that the sharp interface that separates the fluids (which have equal viscosities) is a periodic graph. The flow is two-dimensional and the fluids fill the entire plane.
We reformulate the problem as an abstract parabolic evolution equation for the interface between the fluids and prove local-in-time well-posedness and parabolic smoothing in subcritical Sobolev spaces. Furthermore, we show exponential stability of the zero solution, in the case where gravity effects are neglected.

S15: Uncertainty quantification

Organizer(s): Tamellini, Lorenzo *(CNR-IMATI)*
Lux-Gottschalk, Kerstin *(Eindhoven University of Technology)*

S15.01: Applications of UQ

Date: March 19, 2024 08:30–10:30
Room: G22/105
Chair(s): Lux-Gottschalk, Kerstin

UM-Bridge: Bridging the Gap between Advanced UQ and Advanced Models from Prototype to HPC

Seelinger, Linus (1); Reinarz, Anne (2) 08:30
1: Karlsruhe Institute of Technology
2: Durham University, UK

While deterministic simulation is ubiquitous, UQ remains much less widespread. In particular, the most advanced UQ methods are not routinely applied to computationally challenging numerical models, even though that's where they offer the greatest benefits.

We believe this is largely due to technical complexity and lack of separation of concerns when combining state-of-the-art UQ, models and HPC capabilities.

Addressing these issues, we present UM-Bridge, a language-agnostic software interface for coupling any simulation code to virtually any UQ software. Easy to use integrations for C++, Python, R, MATLAB and Julia as well as several UQ packages like PyMC, MUQ, QMCPy and Sparse Grids Matlab Kit are available.

Inspired by microservice architectures, UM-Bridge enables containerization of models. In a community effort we are building the, to our knowledge, first library of ready-to-run UQ benchmark problems.

Further, UM-Bridge provides platforms for scaling up containerized models on cloud or HPC systems, enabling even prototype-grade UQ applications to offload costly model evaluations to powerful compute clusters.

Finally, we demonstrate the effectiveness of the approach at the example of an HPC-scale UQ application.

Combining noisy well data and expert knowledge in a Bayesian calibration of a flow model under uncertainties: an application to solute transport in the Ticino basin

Baker, Emily (2); Manenti, Sauro (2); Reali, Alessandro (1,2); Sangalli, Giancarlo (1,2); Tamellini, Lorenzo (1); Todeschini, Sara (2) 09:10
1: CNR-IMATI, Italy
2: University of Pavia, Italy

In this talk we present the results of a case-study aimed at providing a UQ analysis of solute travel times in groundwater in the basin of the Ticino River (northern Italy), starting from well data collected over a month in summer 2014.

We consider a steady-state groundwater flow model (developed in MODFLOW) and perform a sensitivity analysis using the Morris method to discard uninfluential parameters. We then employ Bayesian inversion (with Gaussian approximation) to obtain a data-informed posterior pdf for the remaining parameters, and propagate these pdfs to travel times computed by particle tracking (MODPATH).

The likelihood function employed in the Bayesian inversion takes into account both well measurements and expert knowledge about the extent of the springs in the domain under study.

Refs:
E. Baker, S. Manenti, A. Reali, G. Sangalli, L. Tamellini, S. Todeschini
Combining noisy well data and expert knowledge in a Bayesian calibration of a flow model under uncertainties: An application to solute transport in the Ticino basin

GEM - International Journal on Geomathematics, 2023
E. Baker, A. Cappato, S. Todeschini, L. Tamellini, G. Sangalli, A. Reali, S. Manenti
Combining the Morris Method and Multiple Error Metrics to Assess Aquifer Characteristics and Recharge in the Lower Ticino Basin, in Italy.
Journal of Hydrology, 2022

Bayesian data assimilation for complex wetting processes with transport maps and stochastic surrogates

Bonart, Henning (1); Marzouk, Youssef (2)
1: TU Darmstadt
2: Massachusetts Institute of Technology, USA

09:30

Droplets impinging and wetting solid surfaces are ubiquitous in energy, health, or manufacturing applications. For the performance it is important to control how drops impact, stick to, rebound and slide away from solid substrates. Bayesian data assimilation allows to continuously integrate experimental measurements with complex numerical models to improve the estimation of states and parameters. In turn, these accurate estimations can be used for precise control of the drop-solid interaction. However, in the underlying Bayesian inference, evaluating the likelihood function requires very costly simulations of the wetting process.

Therefore, we adopt the measure transport approach to simulation-based inference and construct probabilistic surrogates. We will show how to formulate Bayesian inference with transport maps, train transport maps from joint distributions of parameters and outputs of the stochastic simulation model, and sequentially update the posterior via Bayesian filtering. The costly training phase is conducted offline, while the estimation phase operates near real-time. We demonstrate our approach by estimating parameters and states from artificial noisy data of impacting drops on solid surfaces generated with the complex and accurate Cahn-Hilliard-Navier-Stokes equations.

Scale-bridging within a complex model hierarchy for investigation of an innovative circular energy economy by use of Bayesian model calibration

Gossel, Lisanne (1); Corbean, Elisa (2); Dübal, Sören (3); Brand, Paul (1); Neumann, Jannik (4); Fricke, Mathis (1); Nicolai, Hendrik (5); Stephan, Peter (4); Hasse, Christian (5); Hartl, Sandra (3); Ulbrich, Stefan (2); Bothe, Dieter (1)
1: Institute for Mathematical Modeling and Analysis, TU Darmstadt
2: Nonlinear Optimization Group, Department of Mathematics, TU Darmstadt
3: Optical Diagnostics and Renewable Energies Group, Darmstadt University of Applied Sciences
4: Institute for Technical Thermodynamics, TU Darmstadt
5: Institute for Simulation of reactive Thermo-Fluid Systems, TU Darmstadt

09:50

In search for an energy storage material, which enables future renewable energy supply on a global scale, metal powders recently gain growing interest in energy science and engineering as a recyclable chemical energy carrier [1]. Research on this idea covers a huge range of scales from fundamental materials research on the micro- to nanoscale via mesoscale laboratory and pilot applications to global scale models incorporating economics, logistics and political scenarios [1]. Aiming to make this new technology ready for application in a relatively short time frame, efficient transfer of information within the model hierarchy of different scales and complexities is a challenge in itself. In order to transfer information from the laboratory or pilot reactor scale to the global one, efficient reactor simulations of reduced complexity (i.e. chemical reactor networks, CRNs, [2]) are investigated to be used complementary to Computational Fluid Dynamics (CFD) simulations and experiments, which both yield detailed information but are very expensive concerning time and resources. However, to tap the potential of the efficient CRN method, CRN simulations have to be valid on a denser parameter set than provided by CFD methods. By default, a CRN for a certain parameter set (e.g. operating condition) is constructed based on a respective CFD simulation with the same conditions. Thus, it is not a priori clear if the CRN approach can produce meaningful results for a set of parameters for which no corresponding CFD data exists. Recently, a first attempt to use Bayesian model-to-model calibration for estimating the predictive capacity of CRNs has been developed [3], based on the methods

suggested by Sargsyan *et al.* [4]. In the present contribution, this approach is extended for application in the context of a metal energy cycle. In a parameterized CRN model, uncertain parameters are inferred by Bayesian calibration to a set of CFD data points, and the resulting posterior distributions are used for the prediction of observables. It is investigated if and to what extend the combination of CRNs and Bayesian parameter estimation is suitable for the task of scale-bridging in the context of the metal energy cycle under investigation.

[1] Neumann, J. *et al.* (2023). *Applications in Energy and Combustion Science*, *14*, 100128.

[2] Trespi, S. *et al.* (2020). *Energy & Fuels*, *35*(9), 7121-7132.

[3] Savarese, M. *et al.* (2023). *International Journal of Hydrogen Energy*.

[4] Sargsyan, K. *et al.* (2015). *International Journal of Chemical Kinetics*, *47*(4), 246-276.

Uncertainty of mechanical properties of short-fiber reinforced polymers manufactured by injection-molding process

Rohrmüller, Benedikt (1); Hohe, Jörg (1); Kärger, Luise (2); Beckmann, Carla (1)

1: Fraunhofer IWM
2: Karlsruhe Institute of Technology

10:10

Short-fiber reinforced composites are used in lightweight construction due to their low specific density and high strength-to-weight ratio. In this contribution, the material uncertainty of a composite material is investigated by mechanical characterization and multiscale simulations based thereon. The aim is to assess the propagation of uncertainties across the scales.

The material investigated has a heterogeneous microstructure out of a phenolic-resin polymer matrix reinforced with short-glass fibers. The material was compounded and manufactured in a thermoset injection-molding process at Fraunhofer ICT [1]. Due to the material flow in the manufacturing process, this composite has an uncertainty in the fiber orientation distribution. This leads to an uncertainty in the mechanical properties. In order to characterize the uncertainty of the mechanical properties, large scale tensile, compression and shear tests as well as small scale tensile tests are performed. [2] Finite element simulations of the microstructure are performed to investigate the influence of the scattering of the fiber orientation distribution and the fiber volume content. In addition, they form the basis for multiscale simulations.

Acknowledgement:

The present work has been funded by the Deutsche Forschungsgemeinschaft (DFG, German Research Foundation) under Grant no. 464119659. The financial support is gratefully acknowledged.

Referenzen

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[2] B. Rohrmüller, F. Kneisel, J. Hohe, C. Beckmann, UNCECOMP Proceedings, **2023**.

S15.02: Applications of UQ

Date: March 19, 2024 16:30–18:30
Room: G22/105
Chair(s): Barth, Andrea

Sparse polynomial chaos expansions: a review of recent developments

Sudret, Bruno

ETH Zurich

16:30

Computational models, a.k.a. simulators, are used in all fields of engineering and applied sciences to help design and assess complex systems *in silico*. Advanced analyses such as optimization or uncertainty quantification, which require repeated runs by varying input parameters, cannot be carried out with brute force methods such as Monte Carlo simulation due to computational costs. Thus the recent development of *surrogate models* such as polynomial chaos expansions (PCE).

To cope with the curse of dimensionality, *sparse* expansions have emerged for more than a decade [1] with the introduction of sparse solvers such as least-angle regression. More recently, numerous other algorithms have been proposed. In the first part of this talk, we introduce several solvers and compare their efficiency on various benchmark functions so as to guide users to the best a priori choice [2, 3]. We finally present extensions of PCEs to engineering problems with complex system dynamics, both in the time and frequency domain, introducing the so-called time (resp. frequency) *warping* techniques.

[1] G. Blatman and B. Sudret. Adaptive sparse polynomial chaos expansion based on Least Angle Regression. Journal of Computational Physics, 230:2345–2367, 2011.

[2] N. Lüthen, S. Marelli, and B. Sudret. Sparse polynomial chaos expansions: Literature survey and benchmark. SIAM/ASA Journal on Uncertainty Quantification, 9(2):593–649, 2021.

[3] N. Lüthen, S. Marelli, and B. Sudret. Automatic selection of basis-adaptive sparse polynomial chaos expansions for engineering applications. International Journal for Uncertainty Quantification, 12(3):49–74, 2022.

Advanced Directional Importance Sampling Method for Dynamic Reliability Analysis of Linear Structural Systems under Stochastic Non-Gaussian Loading

Zhang, Xuanyi (1,2); Misraji, Mauricio (2); Valdebenito, Marcos (2); Faes, Matthias (2) 17:10
1: Peking University
2: TU Dortmund University

Reliability analysis of dynamic structural systems and its implications for structural design have garnered increasing attention. A prominent approach for addressing this challenge involves Monte Carlo simulation and its variants. Sample-based methods prove insensitive to the dimension of the probability integral but may necessitate a substantial number of realizations for small failure probabilities, resulting in time-consuming computations.

Recently, the Directional Importance Sampling (DIS) method was introduced for linear structural systems, showcasing the ability to estimate small failure probabilities (e.g., 10^{-3} or less) with a reduced number of dynamic response simulations (e.g., a few hundred). The efficiency of the DIS method hinges on the explicit calculation of dynamic response, capitalizing on the linearity in Gaussian space. However, when the loading is non-Gaussian, which is common in practice, the dynamic response becomes non-Gaussian, and its value in Gaussian space cannot be directly obtained. Consequently, the existing DIS method is not applicable to non-Gaussian problems.

This contribution introduces an advanced DIS method, named DIS+, specifically designed for efficient dynamic reliability analysis of linear structural systems under stochastic non-Gaussian loading. The non-Gaussian dynamic response is simulated using a unified Hermite polynomial model based on its first four moments, enabling the explicit calculation of its associated Gaussian counterpart. With the dynamic response in hand, the DIS procedure can be easily executed in two steps. Firstly, the failure probability at fixed instants is calculated based on the first four moments of the dynamic response. Subsequently, the direction corresponding to the obtained reliability index is analytically determined. In the second step, a few hundred random direction samples are generated according to the importance sampling density function, and the failure probability is calculated based on the corresponding estimator. Notably, sampling is only required in the second step, and the number of samples required is relatively small. Furthermore, the calculation of the reliability index employs an explicit formula, enhancing the efficiency of the DIS+ method. The application of the proposed DIS+ method is illustrated through a series of examples, showcasing its accuracy and efficiency for dynamic reliability analysis.

Efficient model order reduction of vibroacoustic problems under stochastic loads

Hüpel, Yannik; Römer, Ulrich 17:30
TU Braunschweig

In an aircraft, one of the main driving factors of comfort, noise, is influenced by the surrounding turbulent boundary layer (TBL) and other stochastic influences and can be considered early on by

conducting vibroacoustic simulations. Full-scale vibroacoustic simulations of aircraft configurations are challenging due to many reasons, one of them being the vibroacoustic model's size and the entailing computational effort. Model order reduction can help to significantly reduce this computational effort by decreasing the system's size. However, even creating reduced order models (ROMs) can be challenging due to the different stochastic influences stemming from uncertain input parameters and the TBL.

This contribution aims to present an efficient way of constructing ROMs for this task. To this end, we first carry out parametric moment matching to account for the various uncertain material parameters of the model. Then, a low-rank approximation of the stochastic right-hand-side, representing the TBL source, is carried out and the ROM is augmented to provide accurate results for the eigenvectors of the employed Karhunen-Loève expansion. The so-constructed ROM provides efficient approximations of the solutions' mean value and variance, conditional on the material parameters. Since using a full aircraft model is challenging with regards to computational effort, we employ a vibroacoustic benchmark model, consisting of a plate and fluid cavity, to show the benefits of the presented method.

Statistical reduced order modelling for frequency dependent PDEs

Hermann, Lucas; Römer, Ulrich
TU Braunschweig

17:50

The Finite Element Method (FEM) is widely used in the numerical simulation of wave propagation problems. Coupled with measurement data of a real world system, we study a monitoring setting, in which the FEM solution is updated with respect to the data. The statistical FEM (statFEM) can be used to solve the data assimilation problem while quantifying the model-to-reality mismatch. In statFEM, the model state as well as the model-to-reality error are approximated as Gaussian processes (GPs), which yields a Gaussian posterior distribution as well. Contrary to most Bayesian inversion techniques, here the model state is subjected to Bayesian inference, whereas the distribution of the parameters remains unchanged. In the context of state monitoring and data assimilation, there is a need to simulate and assimilate data rapidly, which is particularly challenging if the FEM system of equations is large and the solution needs to be obtained for different frequencies and parameter values. Hence, we introduce a reduced order model (ROM) as an efficient surrogate, which reduces the computation times, albeit inducing an additional ROM approximation error. In particular, we employ a second order Arnoldi moment matching method and we introduce a variant of statFEM which accounts for the ROM error. The ROM error itself is estimated point wise using an adjoint error indicator.

We first illustrate the methods efficiency and the error estimation procedure with a simple 1D example, which is a discretization of the Helmholtz equation with Neumann and impedance boundary conditions. We show that the proposed method is able to approximate the full order statFEM results with a high accuracy, while relying on much smaller systems. As a second example we consider a 2D acoustic scattering problem and again discuss the performance of the method and open research questions.

Towards a Sampling-Free Statistical Finite Element Method in Computational Mechanics

Narouie, Vahab; Wessels, Henning; Römer, Ulrich
TU Braunschweig

18:10

We are investigating the assimilation of sensor data with computational predictions in mechanics via the *statistical finite element method* (statFEM), a novel approach to physics-constrained data regression [1]. Following the statFEM framework, our approach initiates a *stochastic finite element method* (SFEM) incorporating a stochastic material parameter through the *Polynomial Chaos* (PC) technique [2]. Contrary to Bayesian parameter updating [3], in statFEM, the stochastic material parameters remain unchanged. We presuppose a stochastic calibration phase has been completed, allowing our focus to pivot to real-time predictions that leverage sensor data and simulation outputs. We explicitly include consideration of model-reality misspecification as a stochastic process, utilizing the Karhunen-Loeve

expansion, where its stochastic coefficients, referred to as hyperparameters, are updated together with the displacement field.

Our objective is achieved by representing the non-Gaussian stochastic displacement field, the non-stationary Gaussian stochastic model-reality mismatch, and the Gaussian stochastic sensor error as three distinct random fields, each within their suitable PC basis. To update the PC coefficients of the stochastic displacement field, we employ the Gauss-Markov-Kalman filter, an approach introduced in [3]. In the statFEM context, the relationship between the updated entity (the displacement fields) and the observational data is characterized by a linear spatial transformation, aligning well with the linearity prerequisite of this filter.

Utilizing the updated PC coefficients of the displacement field enables the efficient calculation of the mean and covariance of the posterior displacement without extensive sampling. The determination of hyperparameters is carried out by minimizing the negative log marginal likelihood, including a limited Monte-Carlo sampling for the stochastic displacement derived from the PC coefficients of SFEM.

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-Loeve expansion as a lognormal random field. The sampling-free statFEM approach has several advantages; in particular, the displacement can be inferred online. Hence, the method is ideal for digital twinning and structural health monitoring.

References:

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[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.

S15.03: UQ - Multilevel sampling

Date: March 20, 2024 08:30–09:30
Room: G22/105
Chair(s): Lux-Gottschalk, Kerstin

The Quasi Continuous-Level Monte Carlo Method and its Applications

Barth, Andrea; Beschle, Cedric 08:30
University of Stuttgart

The accurate and efficient estimation of moments of (functionals of) solutions to stochastic problems is of high interest in the field of uncertainty quantification. Adding nonlinearities to the underlying stochastic model may lead to large local effects in the solutions and inefficiencies in the moment estimation. Standard multilevel Monte Carlo methods (MLMC) are robust, but not able to efficiently account for these local effects, resulting in high computational cost. The standard continuous level Monte Carlo method (CLMC) can account for local solution features, but with its level distribution sampled by (pseudo) random numbers, it is troubled by a high variance. Thus, we consider the quasi continuous level Monte Carlo method (QCLMC), which combines adaptivity to local solution features via samplewise a-posteriori error estimates with quasi random numbers to sample its underlying continuous level distribution. Therefore, QCLMC has the potential of a high cost reduction and improved performance in comparison to MLMC and standard CLMC, which is demonstrated via applications to random elliptic equations with discontinuous coefficients and to a random inviscid Burgers' equation.

Towards Multilevel Slice Sampling for Bayesian inverse problems
Bitterlich, Kevin; Sprungk, Björn
TU Bergakademie Freiberg 08:50

Slice sampling is a Markov chain Monte Carlo method for drawing (approximately) random samples from a given posterior distribution, which is in general only known up to a normalizing constant. The method is based on sampling a new state on a slice, i.e., a level set of the target density function. Slice sampling is especially interesting because it is tuning-free and we always move to a new state which could result in a lower autocorrelation compared to Metropolis-Hastings, for example. However, to find such a new state can possibly require many evaluations of the target density and thus yield high computational costs.

Therefore, in this talk we introduce the so-called delayed acceptance slice sampler. The idea behind this is that we exploit a cheap approximation to the target density for finding potential new states. We formulate certain properties, illustrate the advantage of the cost reduction in a Bayesian inverse problem and give a result, which shows, that the delayed acceptance slice sampler is theoretically more efficient than the delayed acceptance Metropolis-Hastings algorithm. Moreover, we present an approach for extending our two-level method into a multilevel framework.

A parallel high-performance multi-level Monte Carlo method with memory constraint and CPU-time budget
Baumgarten, Niklas
Karlsruhe Institute of Technology 09:10

We present a parallel high-performance variant of the multi-level Monte Carlo method, designed to operate within a memory constraint and with a specified CPU-time budget. Our approach combines concepts of the continuation multi-level Monte Carlo method with dynamic programming techniques following Bellman's optimality principle, and a new parallelization strategy based on the dynamic assembly of distributed data structures. The algorithm is capable to estimate statistical moments of complete solutions to partial differential equations with random input data. We also show that the algorithm's error reduction adheres to a theoretical bound with respect to CPU-time and provide empirical evidence that our implementation follows the predicted behavior.

S15.04: UQ and dynamical systems

Date: March 20, 2024 14:00–16:00
Room: G22/105
Chair(s): Tamellini, Lorenzo

Dynamical and neural network approaches to downscaling of noisy and partial observations
Knio, Omar
KAUST, Saudi Arabia 14:00

This talk discusses the generation of high-resolution representations through the assimilation of coarse, noisy observations. We consider recently introduced Continuous Data Assimilation (CDA) algorithm, that constructs an increasingly accurate representation of the system states by continuously nudging the large scales using the coarse observations; a Discrete Data Assimilation (DDA) approach that relies on a discrete-in-time nudging scheme; and a physics-informed neural network that is trained to provide a high-resolution forecast based on suitable coarse resolution history. We investigate the performance of all three algorithms for downscaling noisy observations of the Rayleigh-Bénard convection system in the chaotic regime. The CDA solution is shown to converge towards the reference solution faster than that of DDA but at the cost of a higher asymptotic error. The numerical results also suggest a quadratic relationship between the mean-square error and the noise level for both CDA and DDA. The results also suggest that the PINN responds to uncertainties similar to the theorized and numerically-validated CDA behavior, with an additional overhead due to inherent errors in approximating the lifting function.

Bifurcation diagrams of PDEs with parametric uncertainty

Kuehn, Christian; Piazzola, Chiara; Ullmann, Elisabeth 14:40
Technical University of Munich

Complex physical phenomena can often be described by PDEs with random coefficients, possibly involving a large number of uncertain parameters. Crucially, the presence of such uncertainty might render into very different behavior of the modeled phenomenon, e.g. due to the randomness of the stability region of an equilibrium.
In this talk, we consider model equations such as the Allen-Cahn equation with polynomial nonlinearity. We take a look at bifurcation diagrams and regard them as random objects, meaning that e.g. equilibria and bifurcation points are random quantities. As such, they call for uncertainty quantification methods. In particular, we investigate the forward uncertainty quantification problem, i.e. the propagation of the uncertainty of the model coefficients to such quantities by means of sparse grids and the polynomial chaos method.

Koopman Mode Decomposition of a system with uncertain parameters

Gießler, Stephanie; Proppe, Carsten 15:00
Karlsruhe Institute of Technology

In these last years, describing the time evolution of nonlinear systems through the Koopman Operator has gained increased interest. The motivation for doing this lies in the linear nature of the Koopman Operator. However, finding exact representations is challenging since the Koopman Operator has, in general, infinitely many dimensions. Unfortunately, there is no guarantee that an exact finite representation can be found for a particular system. Since it has become known how the Koopman operator can be approximated using data-driven methods, such as eDMD or deep learning-based approaches, this form of description for nonlinear systems has become popular.

This work focuses on the state prediction of systems with uncertain parameters using the Koopman Operator. We base our investigation on simulated data generated through a nonlinear differential equation with uncertain system parameters. To be precise, we use state trajectories of the uncertain system. With that, we investigate how the approximation of the Koopman Operator is affected by the uncertainty in the system parameters. In particular, we study the spectral decomposition, meaning the eigenvalues and eigenfunctions of the approximated Koopman Operators, which is known as the Koopman mode decomposition.

However, the uncertain system parameters are not the only source of uncertainty. While the real Koopman Operator is a global representation of the system, this is not true for its finite-dimensional approximation. Therefore, different initial values of the state trajectories result in different approximations of the Koopman Operator. Finally, we show how these various sources of uncertainties affect the state prediction with the Koopman Operator.

Sensitivity Analysis for Bifurcations in Random Ordinary Differential Equations

Lux-Gottschalk, Kerstin (1); Ashwin, Peter (2); Wood, Richard (3); Kuehn, Christian (4) 15:20
1: Eindhoven University of Technology
2: University of Exeter, UK
3: Met Office Hadley Centre, UK
4: Technical University of Munich

Nonlinear dynamical systems might undergo critical transitions from their current stable state to a drastically different one due to changes in forcing parameters of the system. Equilibria can newly form, cease to exist or change stability properties. We approach these tipping events by applying bifurcation theory of dynamical systems. In real-world scenarios, some system parameters are highly uncertain inducing the need to include uncertain parameters in models of differential equations turning them into random ordinary differential equations. Even a slight misspecification of a model parameter can crucially change the bifurcation structure of the system.

In this talk, I will address impacts of parameter uncertainty on bifurcations in random ordinary differential equations. I will introduce a framework combining sensitivity analysis and bifurcation theory that allows for a quantification of the impact of parameter uncertainties on the bifurcation structure. I will illustrate our methodology for a conceptual climate model of the Atlantic Meridional Overturning Circulation, which is one of the identified earth system tipping elements, and present numerical results on its tipping behavior.

On finite dimensional noise and finite dimensional models in uncertainty quantification
Starkloff, Hans-Jörg 15:40
TU Bergakademie Freiberg

In forward and inverse problems for differential equations with random parameters or random variational inequalities the concept of finite dimensional noise plays a great role. In the talk theoretical difficulties in the use of this concept are adressed. These are for example related to the fact that usual definitions of a finite dimensional noise are not consistent and allow a much wider class of corresponding random functions or random fields.

S15.05: Methodologies for forward UQ
Date: March 20, 2024 16:30–18:30
Room: G22/105
Chair(s): Barth, Andrea

Neural network based operator surrogates for elliptic PDEs
Marcati, Carlo (1); Schwab, Christoph (2); Zech, Jakob (3) 16:30
1: University of Pavia, Italy
2: ETH Zurich
3: Heidelberg University

Approximating solution sets of PDEs is an important task for many applications, e.g., model order reduction and uncertainty quantification. Here, we consider the problem of approximating the solution operator of the PDE, viewed as a map between subsets of infinite dimensional spaces. In recent years, several techniques based on neural networks (NN) have been developed to tackle this problem.
In this talk, I will present some theoretical results on the approximation of solution operators of elliptic PDEs by NN-based surrogates. I will discuss the convergence rates of neural operators and how they vary depending on the smoothness of the coefficients in the input sets. I will then focus on PDEs with lognormal coefficients: in this case, the operator is not uniformly Lipschitz and the error is measured in the mean-square sense, with a Gaussian measure on the input space. The analysis of this case relies on (novel) sparsity estimates for the solutions and on the NN emulation of Hermite polynomials.

Adaptive multilevel Neural Networks for parametric PDEs with error control
Eigel, Martin; Schütte, Janina 17:10
Weierstrass Institute for Applied Analysis and Stochastics

We present multilevel neural networks for high-dimensional parametric PDEs. The architecture consists of U-Net CNNs, which reflects the notion of multigrid algorithms as known from finite elements. In fact, the convergence analysis relies on the observation that CNNs can represent all components of a multigrid algorithm efficiently, leading to favourable convergence results. Based on a hierarchy of nested meshes, the neural network training exploits the multilevel properties of the data, reducing the overall effort and resulting in excellent practical performance.

We extend this architecture by also learnnig a reliable a posteriori error estimator that provides error bounds on the layerwise approximation error. Training data is generated with an adaptive finite element method, leading to local mesh refinements that are reflected in the CNN by culling masks. This leads to further efficiency improvements that are illustrated with benchmark examples.

Adaptive sparse grid methods with kink detection for uncertainty quantification in gas networks

Wilka, Hendrik; Lang, Jens 17:30
TU Darmstadt

Uncertainty quantification plays an important role in the simulation and optimal control of gas networks. In our models, we allow the demands of consumers to be uncertain and investigate the probability that certain pressure bounds are satisfied in the network. Even in small networks, we can observe the formation of kinks for certain quantities of interest computed from approximate solutions. Hence, we need an accurate approximation of high-dimensional functions with kinks and their integrals.

We consider approximations on sparse grids with local refinements, where we use local polynomials with a restricted support as multilinear basis functions. Fundamental work in this area was done by Bungartz who introduced the idea of using ancestor nodes outside the support of basis functions to achieve higher polynomial degrees [1998, Habilitationsschrift]. This works well if sufficient smoothness of the high-dimensional function can be assumed, but functions with kinks are challenging to approximate. Ma and Zabaras used local linear basis functions to address this problem [2009, J. Comput. Phys. 228], while Jakeman and Roberts [2011, arXiv:1110.0010v1] investigated the use of high-degree basis functions in this setting.

We provide a novel hp-generalised sparse grid algorithm which combines both approaches. We allow high-degree local polynomial basis functions, but our algorithm chooses the polynomial degree for each one-dimensional basis function individually. Hence, low polynomial degrees can be chosen near kinks, while higher degrees are used in smooth regions to achieve faster convergence.

Two main strategies to find suitable polynomial degrees for the basis functions are presented: The first one uses a greedy approach which selects the basis with the best interpolation properties at certain test points. The second strategy incorporates a kink detection algorithm to refine in non-smooth regions (h-refinement) and to increase the polynomial degree in smooth areas
(p-refinement).

We will compare our approach with existing methods. We first look at toy problems and then discuss gas network problems.

Application of Isogeometric Analysis for Interval Analysis

Manque, Nataly; Liedmann, Jan; Barthold, Franz-Joseph; Valdebenito, Marcos; Faes, Matthias 17:50
TU Dortmund University

Geometrical uncertainty poses a significant challenge in manufacturing processes, often attributed to the underlying manufacturing technology and operating conditions. When combined with geometric complexity, this phenomenon can result in substantial disparities between numerical predictions and the actual behavior of mechanical systems. The underlying cause lies in the initial design phase, where insufficient information impedes the development of robust numerical models due to epistemic uncertainty in system dimensions. In such cases, set-based methods, like intervals, prove useful for characterizing these uncertainties by employing lower and upper bounds to define uncertain input parameters. Nevertheless, employing interval methods for treating geometric uncertainties can become computationally demanding, especially when traditional methods like finite element (FE) are utilized to represent the system and propagate uncertainty. This is due to the necessity of performing iterative analyses for different realizations of geometry within the bounds of uncertain parameters, requiring the repeated execution of the meshing process and thereby escalating the numerical effort. In this work, the potential of Isogeometric Analysis (IGA) for quantifying geometric uncertainties characterized by intervals is explored. IGA utilizes the same basis functions, Non-Uniform Rational B-Splines (NURBS), employed in Computer-Aided Design (CAD) to approximate solution fields in numerical analysis. This integration enhances the accurate description of complex shapes and interfaces while maintaining geometric fidelity throughout the simulation process. The primary advantage of employing IGA for uncertainty quantification lies in its ability to control the system's geometry through the position of control points, which define the shape of NURBS. Consequently, alterations

in the model's geometry can be achieved by varying the position of these control points, thereby bypassing the numerical costs associated with uncertainty quantification using intervals. To propagate geometric uncertainties, a gradient-based optimization algorithm is applied to determine the lower and upper bounds of the system response. The corresponding sensitivities are computed from the IGA model. A case study involving a linear hook system with two uncertain geometric parameters demonstrates that the proposed strategy accurately estimates uncertain stress triaxiality.

Unlocking Possibilities: Quantifying Imprecise Probabilities with Possibility Theory
Könecke, Tom; Hanss, Michael
University of Stuttgart
18:10

In the realm of engineering, there is a need for accurately addressing and faithfully quantifying uncertainties. This contribution aims to motivate the use of imprecise probabilities for uncertainty quantification, emphasizing the vital distinction between aleatory uncertainties, which are random and unavoidable, and epistemic uncertainties, which stem from limited data or knowledge. Epistemic uncertainty, in particular, presents a significant challenge in engineering, necessitating innovative approaches for appropriate quantification and effective propagation, where the classical probabilistic framework often turns out to be inadequate.

A potential solution to this challenge lies in the domain of imprecise probabilities, which encompass methodologies like p-boxes and Dempster-Shafer theory among others. These methods provide a robust framework for dealing with incomplete information, thereby enhancing the precision of uncertainty quantification.

This contribution advocates the concept of possibility theory as a theory of imprecise probabilities. Possibility theory offers a robust and surprisingly trivial approach to quantifying uncertainties, where the dual possibility and necessity measures serve as probability bounds. The theory stands out for its ability to handle polymorphic uncertainty effectively, while ensuring reliable and inclusive results in engineering analyses as well as in decision-making. A key advantage of the here presented view of possibility theory is its close relation to the theory of fuzzy arithmetic, which by dint of some specific adjustments provides a solid basis for the efficient implementation in engineering applications.

Novel developments over the last few years extend the applicability of possibility theory to various practical scenarios, providing a robust methodological framework for data inference and transformation. The so-called Imprecise-Probability-to-Possibility-Transform facilitates the integration of different types of information, ranging from expert knowledge via sparse data to precise probability distributions, into a cohesive analytical model and actionable insights.

However, the field of possibility theory and imprecise probabilities is not without its challenges. Future research directions include remaining computational challenges and further pursuit into the idea of partial priors. This contribution aims to shed light on these challenges and potential developments, thereby contributing to the advancement of imprecise probabilities as a practical tool for uncertainty quantification in engineering.

S15.06: UQ - Sampling and rare events estimation

Date: March 21, 2024 08:30–10:30
Room: G22/105
Chair(s): Tamellini, Lorenzo

Consensus-Based Rare Event Estimation
Ullmann, Elisabeth
Technical University of Munich
08:30

We introduce a new algorithm for rare event estimation based on adaptive importance sampling. We consider a smoothed version of the optimal importance sampling density, which is approximated by an ensemble of interacting particles. The particle dynamics is governed by a McKean-Vlasov stochastic differential equation, which was introduced and analyzed in [Carrillo et al., Stud. Appl. Math.

148:1069-1140, 2022] for consensus-based sampling and optimization of posterior distributions arising in the context of Bayesian inverse problems. We develop automatic updates for the internal parameters of our algorithm. This includes a novel time step size controller for the exponential Euler method, which discretizes the particle dynamics. The behavior of all parameter updates depends on easy to interpret accuracy criteria specified by the user. We show in numerical experiments that our method is competitive to state-of-the-art adaptive importance sampling algorithms for rare event estimation, namely a sequential importance sampling method and the ensemble Kalman filter for rare event estimation.
This is joint work with Konstantin Althaus and Iason Papaioannou (TUM).

Computing upper probabilities of failure using optimization algorithms together with importance sampling.

Fetz, Thomas; Oberguggenberger, Michael 09:10
University of Innsbruck

In reliability analyis the combination of probabilistic and non-probabilistic methods has become an important issue. In particular, the uncertainty about the values concerning properties of an engineering structure can be modelled by a family of probability density functions parametrized by all t in a set T. The output of such a model typically consists of upper and lower probabilities, for example, the upper failure probability, which is the solution of a (global) optimization problem max $p(t)$: t in set T where $p(t)$ is the failure probability for a fixed parameter value t. We estimate these function values $p(t)$ using Monte Carlo simulation which means function evaluations (finite elements computations) for each of N sample points. This high computational effort has to be multiplied in addition by the number of function evaluations $p(t)$ needed for solving the above optimization problem to find the parameter t in T resulting in the upper probability.

To reduce the number of parameter values t for which new samples are required in the optimization algorithm and to reduce sample sizes N itself for such t we re-use the samples generated for parameter$t$ of previous optimization steps [1,2]. For this purpose we take the arising importance sampling ratios into account. This leads to importance sampling on sets of a partition of the space of the uncertain properties of the engineering structure [3]. The above method is combined with strategies for finding good importance sampling densities including the design point to reduce the variance.

The efficiency of this new method is demonstrated by means of a moderate scale engineering problem.

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Probabilistic microstructural modelling of the failure initiation process in cast iron

Beckmann, Carla; Rohrmüller, Benedikt; Schober, Michael; Tlatlik, Johannes; Varfolomeev, Igor; Hohe, Jörg 09:30
Fraunhofer IWM

Cast iron with ferritic matrix and globular graphite inclusions is a common engineering material used in many applications. Their fracture initiation and failure process is strongly controlled by their microstructure consisting of an iron matrix with randomly distributed graphite inclusions. Due to the uncertain microstructure, uncertainties develop in their fracture toughness, thus requiring a probabilistic failure assessment.

The present contribution is concerned with a probabilistic multiscale failure analysis of cast iron wit a mostly ferritic matrix and randomly distributed globular graphite inclusions, utilizing a combined experimental and numerical approach. In a first step, the facture and failure behavior of a selected reference material is characterized experimentally. Based on the experimental observations, a probabilistic multiscale simulation of the fracture process is performed to gain a deeper understanding of the fracture process. The multiscale simulation is based on the analysis of the crack initiation and initial propagation process in stochastic volume elements consisting in detailed models of the direct neighborhood of a pre-existing crack, embedded in a larger volume of the effective material. The microstructure of the stochastic volume elements is generated in a random process based on the experimental observations on the microstructural uncertainty in the first step. As a result of the stochastic multiscale analysis, the uncertainty to be expected in the fracture toughness is analyzed and correlated to the microstructure. The approach is validated against the experimental data base from the first step.

Based on the first two steps, continuum mechanics concepts for integrity assessment are derived and implemented.

Less interaction with forward models in Langevin dynamics: Enrichment and Homotopy

Eigel, Martin (1); Gruhlke, Robert (2); Sommer, David (1)
1: Weierstrass Institute for Applied Analysis and Stochastics
2: FU Berlin

09:50

Ensemble methods have become ubiquitous for the solution of Bayesian inference problems. State-of-the-art Langevin samplers such as the Ensemble Kalman Sampler (EKS) or the Affine Invariant Langevin Dynamics (ALDI) rely on successive evaluations of the forward model or its gradient.
A main drawback of these methods hence is their vast number of required forward calls as well as their possible lack of convergence in the case of more involved posterior measures such as multimodal distributions.
The goal of this paper is to address these challenges to some extend. First, several possible adaptive ensemble enrichment strategies that successively enlarge the number of particles in the underlying Langevin dynamics are discussed that in turn lead to a significant reduction of the total number of forward calls. Second, analytical consistency guarantees of the ensemble enrichment method are provided for linear forward models. Third, to address more involved target distributions, the method is extended by applying adapted Langevin dynamics based on a homotopy formalism for which convergence is proved.
Finally, numerical investigations of several benchmark problems illustrates the possible gain of the proposed method, comparing it to state-of-the-art Langevin samplers.

Modelling Distributions with Wasserstein Proximal methods and Low-Rank Tensor Decompositions

Aksenov, Vitalii; Eigel, Martin
Weierstrass Institute for Applied Analysis and Stochastics

10:10

Minimization in the Wasserstein space gives a framework for sequentially constructing approximations to complicated distributions, which may arise from applications such as Bayesian inversion, importance sampling and generative modelling. For high dimensional problems, Eulearian methods are not usually used, because in general, they suffer from the curse of dimensionality. In the current talk, we attempt to "rehabilitate" the Eulerian methods in high dimension by using the developments in low-rank Tensor Train decomposition. The approach is based on the Fisher Information regularization of the dynamic JKO scheme. This essentially is a proximal step with respect to the Wasserstein distance and can be viewed as a generalization of the implicit gradient descent method to the metric space. The nonlinear transformation of variables allows to represent the problem as a system of heat equations with nonlinear coupling in the initial and terminal condition. The system is formulated as a fixed-point equation, and we explore the possibility of solving it with accelerated methods. An ODE governing the evolution of particles can be defined with help of intermediate variables, giving a deterministic sampling algorithm for the approxinate distribution.

S16: Optimization

Organizer(s): Herberg, Evelyn *(Heidelberg University)*
Kahle, Christian *(University Koblenz)*

S16.01: Topology Optimization I

Date: March 19, 2024 08:30–10:30
Room: G22/110
Chair(s): Kahle, Christian
Herberg, Evelyn

Stabilization of topology optimization problems using Voronoi tessellations

Kikis, Georgia (1); Sauren, Bjorn (2); Birk, Carolin (1); Klinkel, Sven (2)
1: University of Duisburg-Essen
2: RWTH Aachen University

08:30

Topology optimization, which is widely used in mechanical and aerospace engineering, has found its way into civil engineering. The progress made in additive manufacturing as well as new high-performance materials allow for the construction of novel and complex geometric designs. Polygonal elements allow for a more flexible mesh generation and proper representation of these complex-shaped design domains as well as their optimized versions. Additionally, local *h*-refinement can be employed efficiently. In this contribution Voronoi tessellations are used, which represent a highly efficient discretization technique that enables the polygonization of any structure. However, special finite element formulations have to be introduced due to the polygonal element geometries.

The focus in this contribution lies on the determination of a structure's optimal material distribution, while maximizing its stiffness, i.e. minimizing its compliance. The topology optimization problem is analogous to a mixed variational problem and shows the same numerical instability, known as checkerboarding. In this case, in certain regions, void and solid elements are alternating. It is shown that the use of polygonal finite elements with Voronoi tessellations avoids this phenomenon and leads to stable solutions. Several numerical examples are considered and the results are compared to the standard finite element formulation using quadrilateral elements, which are polluted by spurious checkerboard modes.

Shape Design Optimization of a flat Endmill Tool

Kalu-Uka, Abraham (1); Moerman, Kevin (2); Eberhard, Peter (1)
1: University of Stuttgart
2: University of Galway, Ireland

09:10

Among the many possible metal-cutting processes, milling is regarded as one of the most widely applied processes to machine different engineering materials productively. During the milling process, there is relative motion between the endmill tool and the workpiece. Energy is required to drive the cutting force used by the tool in separating the chips from the workpiece. Several studies have focused on the effects of milling process parameters on the cutting force, for instance by varying the cutting parameters, machining properties, and the extent of cooling/lubrication. Other studies have explored the influence of tool geometry and material properties on the cutting force. Results from these studies have brought about improvements in the design of milling machinery and tools. The current study presents a novel automated approach for tool geometry optimization which is fully coded in MATLAB. An automated and parameterized endmill design procedure was created featuring input parameters such as rake angle (face), relief angle (side), clearance angle (side), and helix angle, all of which have been shown, through numerous studies, to influence cutting forces. The parameters were here used to generate the shape profile for one cutting edge of a flat endmill. In particular, the parameters define a set of control points for a smooth cubic spline spanning from the end of the rake face's untipped side to the beginning of the clearance side (moving from right to left). This single cutting edge profile is next copied and rotated, as per the design's pitch angle, to form the complete set of cutting flutes for the flat endmill. Next the surface defined by the completed profile is meshed

using quadrilateral elements. The 3D endmill design is then formed by extruding, and twisting as per the helix angle, this quadrilateral mesh to form a solid hexahedral mesh. Finally, an automated iterative optimization process was defined, featuring the above parameterized design process coupled with Abaqus-based finite element simulation of the milling process. The expected result is that the proposed optimization procedure will be able to identify the endmill design parameters which minimize the cutting force. Furthermore, it is anticipated that the automated design, meshing, and simulation-driven optimization approach is generalizable to other tool design variations.

Remarks on Shape Sensitivity Analysis of Dynamic Structures

Ghasemi, Seyed Ali; Liedmann, Jan; Barthold, Franz-Joseph 09:30
TU Dortmund University

Efficient and lightweight production in design processes relies on structural optimization, where sensitivity analysis plays a crucial role. This study focuses on analytical sensitivity analysis for time-dependent structural behavior. Specifically, the design sensitivity formulations for the direct differentiation method (DDM) [1], [2] and the adjoint variable method (AVM) [3] are explored and compared. DDM and AVM are two techniques to obtain sensitivity information e.g. in structural optimization. DDM computes sensitivities by directly differentiating the structural response equations concerning design variables. However, it requires solving additional equations for each design variable, resulting in computational expenses, especially for large-scale problems. Despite this drawback, DDM's straightforward implementation suits problems with relatively few design variables. Conversely, AVM offers an efficient alternative by utilizing adjoint equations to compute sensitivities, significantly reducing computational costs compared to DDM, particularly for problems with numerous design variables.
The utilization of Isogeometric Analysis (IGA) [4] in structural optimization eliminates costly remeshing and design velocity field calculations. IGA's precise geometry description with fewer control points, high-order continuity, and increased flexibility due to control point weights present advantages over conventional Finite Element Method (FEM) approaches. These properties significantly impact shape sensitivity analysis.
This study compares and discusses the advantages and limitations of both DDM and AVM methods using IGA for analyzing time-dependent structural behavior in shape sensitivity analysis.

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Analysing sensitivity information of composite laminate shell structures

Liedmann, Jan (1); Barthold, Franz-Joseph (1); Nikolai, Gerzen (2) 09:50
1: TU Dortmund University
2: Ostwestfalen-Lippe University of Applied Sciences and Arts

In strucutral optimization of composite laminate shell structures, various goal functions are desired depending on the structure's actual use case. This holds also true for the choice of design parameters as in some cases changes in the fiber orientations are intended without changing the thickness

of the structure at all, while in other cases only specific layer thicknesses and possibly also their fiber orientations may be varied. In this study, basic types of design parameters for composite laminates are investigated, that is, total thickness, specific layer thicknesses, as well as fiber orientations, and sensitivity relations are derived.
The solid shell formulation is based on [1]. On this basis both, an extension to anisotropic material behaviour, cf. [2], as well as the sensitivity relations w.r.t. the shell geometry, cf. [3], has been investigated on in the past years. In this work, these methods have been combined and further developed so as to derive formulations for efficient sensitivity analysis. Based on a variational approach embedding sensitivity analysis into the continuum mechanical framework, sensitivity relations w.r.t. layer thicknesses and fiber orientations are derived. These continuously derived quantities can then easily be discretized and implemented into a finite element environment.
By reference to chosen numerical examples, different aspects, such as computational perfomance, numerical accuracy and algorithmic treatment are discussed comparing different layering models.
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Prediction of CO2 uptake on activated carbon by artificial neural networks

Venturella, Suzan; Brusamarello, Claiton Zanini; de Souza, Fernanda Batista
Federal University of Technology – Paraná, Brazil

10:10

In 2022, CO_2 levels in the atmosphere reached the mark of 420 ppm and became a concerning matter among the scientific community. Climate change may cause, in an indirect way, adverse effects on people's health. Thus, the investments foreseen in the Paris Agreement are essential to reducing the impacts caused by climate change, and it also gives the countries involved the opportunity to develop new technologies to mitigate CO_2 emissions. Carbon capture is one of these technologies, and a technique that can be used is gas adsorption on solid surfaces. To study the uptake of CO_2 on activated carbon under different experimental conditions, this work uses artificial neural networks (ANN) feed with experimental data collected by scientific work (1995-2022) with the use of the Levenberg-Marquardt algorithm for optimization of the network. For training the ANN data of pressure and temperature of the process and the superficial area of the adsorbent were used as inputs. The Matlab® software was used to train the ANN, and the data was distributed as 70% for training, 15% for validation, 15% for testing and trained for 10, 15, and 20 layers. For the use of the collected data, it was necessary to normalize to the range of [-1,1] using the min-max method due to the activated functions used in the network. The network comprises the tangent activation function in the hidden layers and the linear function in the output layer. The mean squared error and the correlation coefficient were used to analyze the outputs obtained through the network test. The best result was obtained for the 20-layer training presenting 215 epochs, MSE equivalent of $2.2x10^{-3}$ and an R^2 of 0.99155 for the training data, 0.98521 for the validation data, 0.98495 for the test data. Therefore, ANNs can model complex relationships, dependent on multiple factors and non-linear in adsorption systems.

S16.02: Topology Optimization II

Date: March 19, 2024 16:30–18:30
Room: G22/110
Chair(s): Kahle, Christian
Herberg, Evelyn

Sequential topology optimization for additive manufacturing

Jantos, Dustin Roman; Kick, Miriam; Junker, Philipp 16:30
Leibniz University Hannover

With modern additive manufacturing techniques, manufacturing of topology optimized structures became more in accessible. Common optimization approaches do not take into account the sequential manufacturing those structures or for large scale structures an assembly of optimized substructures, i.e. the design of a structure is optimized as one closed geometry.

To improve producibility of those structures, we introduce a sequential topology optimization approach in which the limited range of the manufacturing machine, e.g. a robot arm or crane, and/or size of preproduced substructures is accounted for. In this sequential topology optimization approach, the design space is limited according to the working-range of the manufacturing machine and is gradually increased, resulting in multiple separated production steps or optimized substructures. Besides the structural weight, the weight of the manufacturing machine at its position during manufacturing or assembly of the next substructure segment is applied. Thus, the optimization yields step by step new structural parts which are optimal to bear their weight and the weight of the manufacturing machine during production of the next segment. Structural parts, which were established during former optimization steps, are not allowed to be removed. This results in the optimization of the extension of the structure part by part without removing (supporting) structures from previous production steps.

For the topology optimization, we apply the thermodynamic topology optimization approach. The thermodynamic topology optimization is based on Hamilton's principle which yields a closed set of partial differential equations for the mechanical equilibrium and the optimization itself. The solution of the partial differential equation for the optimization converges towards to optimal design and thus serving as optimization algorithm. The set of equations is solved in a staggered approach for maximum numerical efficiency: the balance of linear moment is solved by means of classical finite element method whereas the partial differential equation describing the optimization of the design are solved with a meshfree finite difference scheme.

To this end, the thermodynamic topology optimization under self-weight is introduced and numerical examples for a two-dimensional, sequentially manufactured bridge for varying material- and manufacturing machine weights are presented.

An experimental validation of optimized structures with hardening material behavior

Kick, Miriam; Junker, Philipp 16:50
Leibniz University Hannover

In this talk we present a numerically efficient material model for the consideration of hardening material behavior within our thermodynamic topology optimization. As expected, the optimized structures differ for different types of hardening. The material parameters for the material model are easily identified by simple tensile tests. To validate our method, we develop boundary value problems that result in optimized specimen which can be tested experimentally. The optimized specimens are additively manufactured and compared against an elastic optimized reference. The acquired test data confirm the influence of the material on the structural behavior and consequently the need for its consideration during optimization.

On varying time integration schemes for a density-based topology optimization approach at large deformations

von Zabiensky, Max; Jantos, Dustin R.; Junker, Philipp 17:10
Leibniz University Hannover

Hyperelastic hinges or joints are of increasing interest for specific applications, where individual parts can fulfill the function of an entire assembly. The design of such components is challenging in individual cases and topology optimization may provide a first approach for a more accessible design. To this end, we apply the thermodynamic topology optimization, which is a continuous density-based approach. Herein, the optimization is carried out by the solution of partial differential equations via

a meshfree finite difference while the displacement-field is determined by classical finite element approach (FEM). With regard to the function of the hinge, there are large deformations, especially in the context of a continuous density-based approach, and therefore snap-back and snap-through must be taken into account when solving the FEM. When solving the FEM, the Newton-Raphson algorithm including an arc-length method is used to approximate the non-linear problem, which results in multiple iteration steps within multiple load or time steps. Thus, the update for the design variables within the topology optimization can be applied at different times: within each Newton-Raphson increment or after each load step or only after the load step. The optimization in the last converged load step, i.e., based on the final deformation, is of course independent of the convergence speed or the number of load steps. The deformation history is therefore not relevant in this case. Three approaches are applied for this purpose, which are based on the solution steps mentioned above:

- optimization after each Newton-Raphson loop
- optimization after each load step (with adapted number of increments)
- optimization after the converged final load step

These approaches are examined for varying (adaptive) load increments regarding their computational performance and achieved optimally. Numerical results are presented.

Topology Optimization of Continuum Structures using Simultaneous Stress and Displacement Constraints

Rutsch, Felix (1); Fina, Marc (2); Freitag, Steffen (2); Weeger, Oliver (1)
1: TU Darmstadt
2: Karlsruhe Institute of Technology

17:30

A structural topology optimization approach is presented considering stress and displacement constraints. This is motivated by structural engineering applications. In general, different types of constraints can be considered by global or local measures. However, local stress and displacement constraints represent common engineering problems most closely and allow for a wide variety of applications, especially taking different displacement limits for different structural regions into account. To address this multiconstrained formulation, the optimization process for stress constraints based on the Augmented Lagrangian method is extended for the simultaneous integration of displacement constraints. The corresponding gradient can be derived such that the optimization can be performed using a steepest descent method. Further, the implementation of multiple load cases is discussed. This leads to a highly modular approach that can easily be adapted to different engineering problems. To investigate the effectiveness of this approach, examples of an L-shaped structure and a two-span beam are presented.

Cavity Shape Optimization in Injection Molding to Compensate for Shrinkage and Warpage

Tillmann, Steffen (1); Elgeti, Stefanie (1,2)
1: RWTH Aachen University
2: TU Wien

17:50

In injection molding, shrinkage and warpage lead to shape deviations of the produced parts with respect to the cavity. Caused by shrinkage and warpage, these deviations occur due to uneven cooling and internal stresses inside the part. One method to mitigate this effect is to adapt the cavity shape to the expected deformation. This deformation can be determined using appropriate simulation models, which then also serve as a basis for determining the optimal cavity shape.

We formulate an optimization problem to find the optimal cavity shape. The objective function measures the difference between the desired geometry and the warped geometry. This difference is computed by taking the average Euclidean distance of sample points on the surface of the deformed product on the one hand and the desired shape on the other hand. For the shape adaption we use free-form-deformation, which is a spline-based method, where the geometry is deformed based on

the position of spline control points. Thus, the optimization parameters are the coordinates of the spline points which represent our geometry.

Additionally, we undertake a comparative evaluation of various methodologies for determining the optimal cavity shape, focusing on computational efficiency and effectiveness of the method.

The material parameters can underlie fluctuations due to different batches or when using recycled material. These uncertainties in the material parameters should be accounted for, such that the optimal shape results in low shrinkage and warpage as well as low variance with respect to the input parameters.

Sustainability in bridge design – investigation of the potential of topology optimization and additive manufacturing on a model scale

Masarczyk, Daniela; Arold, Tizian; Niendorf, Thomas; Kuhl, Detlef 18:10
University of Kassel

In the context of sustainable construction in civil engineering and considering the increasing cost of building materials, the design of resource-efficient structures is a key challenge. Mechanical efficiency in structural design ensures that the building materials are used where necessary to support a given load. The design process can be assisted by numerical structural optimization. The manufacturability of optimized structures represents a challenge due to their free, usually non-rectangular shape.

Aim of the present study is to investigate the potential of additive manufacturing (AM) for the realization of optimized bridge models. Bridges are subject to high structural loads, a large part of which is induced by the self-weight of the bridge and therefore needs to be considered in the design process. Numerical topology optimization with consideration of self-weight is used to design the structural layout. Objective of the optimization is structural stiffness with a bound on the disposable amount of material. The popular SIMP method [1], modified for consideration of self-weight [2], is used to interpolate the material stiffness. The highly non-linear optimization problem is solved by a custom topology optimization routine [3] that is based on Sequential Quadratic Programming [4] and written in Matlab. The optimized structural layouts are transferred to a CAD model to enable fabrication by AM.

The optimization results show a strong similarity to already existing arch bridges. A support structure based on an inverted catenary is observed in the resulting structures. The arch and the bridge deck are connected by structures that are likewise subjected to their own weight; therefore, their shape is also based on the catenary which represents a new feature to be incorporated in bridge design. A prototype of an optimized bridge will be manufactured on a small scale by means of a Powder Bed Fusion technique. The bridge models are presented and examined, structural design and the potential of AM for the fabrication of optimized structures in civil engineering are evaluated.

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S16.03: Nonsmooth Problems I

Date: March 20, 2024 08:30–09:30
Room: G22/110
Chair(s): Herberg, Evelyn
Kahle, Christian

Semismooth Newton Methods for Minimization Problems with Box-Constraints in Sobolev Spaces

Christof, Constantin (1); Wachsmuth, Gerd (2)
1: Technical University of Munich
2: BTU Cottbus-Senftenberg

08:30

This talk is concerned with generalized differentiability properties of solution operators of unilateral and bilateral elliptic obstacle-type variational inequalities. We prove that such operators are Newton differentiable with values in the energy space when equipped with a suitably defined computable generalized set-valued derivative. It is shown that this Newton differentiability allows to solve optimal control problems with H01-cost terms and pointwise control constraints of box type by means of a semismooth Newton method. The q-superlinear convergence of the resulting algorithm is established in the infinite-dimensional setting and its mesh independence is demonstrated in numerical experiments. The talk concludes with comments on further applications of the derived results in the context of quasi-variational inequalities and the optimal control of contact problems.

Sparse representation recovery in convex optimization through a metric non-degenerate source condition

Carioni, Marcello; Del Grande, Leonardo
University of Twente, The Netherlands

09:10

In this contribution we analyze the recovery of the sparse representation of data in general infinite-dimensional optimization problems regularized by convex functionals. By assuming a suitable non-degeneracy condition on the dual certificate of the problem we establish that, for small regularization parameters and in a low-noise regime, the minimizer is unique and is uniquely represented as a linear combination of n extreme points of the ball of the regularizer. Such non-degeneracy condition extends to general convex optimization problems the classical non-degeneracy source condition (NDSC) introduced by Duval and Peyré in the context of total variation regularized deconvolution problems. More precisely, it provides conditions on the behaviour of the dual certificate when evaluated on the set of extreme points of the ball of the regularizer, seen as a metric space. This justifies the name Metric Non-Degenerate Source Condition (MNDSC). Due to the lack of differential structure of the set of extreme points, the MNDSC is defined by imposing that the second derivative of the dual certificate is different from zero along parametrized curves in the extreme point set.

Building on our general result, we obtain explicit formulations of the MNDSC, which lead to specific results of sparse recovery for the following three problems of interest. First, we recover a variant of the classical result by Duval and Peyré for total variation regularized deconvolution problems. Then, we analyze the sparse recovery of 1-dimensional BV functions regularized with their BV-seminorm, showing that in this case the MNDSC reduces to a first order condition on the dual certificate evaluated at the jumps of the data. Finally, we consider pairs of measures regularized with their mutual 1-Wasserstein distance, showing that in this case the MNDSC can be rewritten in terms of the Hessian of a suitable functional constructed based on the dual certificate of the problem.

This contribution is based on the preprint (https://arxiv.org/abs/2311.08072), joint work with Leonardo Del Grande.

S16.04: Shape and Topology Optimization

Date: March 20, 2024 14:00–16:00
Room: G22/110
Chair(s): Herberg, Evelyn
Kahle, Christian

Application of a Projection type method on Shape and Topology Optimization Problem concerning Additive Manufacturing

Urmann, Maximilian; Blank, Luise 14:00
University of Regensburg

One main goal of topology optimization is to find an optimal distribution of multiple materials in a design domain in such a way that it can withstand internal and external loads applied on the structure.

Additive manufactuing techniques like 3D-printing are able to produce complex structures and topologies. To guarantee constructability overhangs need either support structures or should be avoided in total.

Using a phase field approach we include this restriction, by studying a control problem minimizing the weighted sum of the Ginzburg-Landau energy with the mean compliances of the whole structure and of each individual layer. To this end, we introduce multiple linear elasticity equations as state equations describing the displacement of the structure to the applied loads.

To solve this problem numerically, the VMPT (Variable Metric Projection Type) method is presented and applied.

Finally, we perform numerical experiments on multiple examples. The impact of model parameters on the shape and topology is discussed. Furthermore the enormous speed up with the VMPT method using variable metrics including second order information is presented.

Mesh-independent topology optimisation in the H^1 Sobolev space

Habera, Michal (1); Hale, Jack (2); Neumann, Johannes (1) 14:20
1: Rafinex SARL
2: University of Luxembourg

Topology optimization for minimal elastic compliance is typically formulated using discontinuous L^2 density fields. Without further modifications, the resulting optima are mesh-dependent and show artifacts such as checkerboarding. To fix these issues, heuristic density and sensitivity filters were introduced in the literature. In this work we present a consistent formulation for H^1 density field topology optimization by interpreting the problem in an infinite-dimensional Hilbert space setting equipped with a weighted norm. Through two-dimensional numerical examples we demonstrate that this formulation produces mesh-independent designs, bounded optimisation iteration numbers, and that the design feature size can be controlled independently of the mesh size.

Convergence of a steepest descent algorithm in shape optimisation using W1,∞functions

Deckelnick, Klaus (1); Herbert, Philip (2); Hinze, Michael (3) 14:40
1: Otto von Guericke University Magdeburg
2: University of Sussex, UK
3: University of Koblenz

We present a general shape optimisation framework based on the method of mappings in the W1,∞topology together with a suitable finite element discretisation. For the numerical solution of the respective discrete shape optimisation problems we propose a steepest descent minimisation algorithm with Armijo-Goldstein stepsize rule. We show that the sequence generated by this descent method globally converges, and under mild assumptions also, that every accumulation point of this sequence is a stationary point of the shape functional. Moreover, for the mesh discretisation parameter tending to zero we under mild assumptions prove convergence of the discrete stationary shapes in the Hausdorff complementary metric. To illustrate our approach we present a selection of numerical examples for PDE constrained shape optimisation problems, where we include numerical convergence studies which support our analytical findings.

A differential geometric point of view on shape optimization

Pryymak, Lidiya; Welker, Kathrin
TU Bergakademie Freiberg

15:00

The design of structures plays a crucial role in many everyday problems. These include medical applications, such as the design of cardiovascular stents and engineering applications, like the construction of aerodynamic wings. Hereby, optimal designs can be derived using a shape optimization formulation of the problem. The underlying shape space, i.e., a space in which each element is given by a shape, should be selected with care, as its properties have a great impact on the optimization algorithm. Often, it is convenient to choose the shape space as a Riemannian manifold and thus the optimization algorithm is based on techniques from differential geometry.

In this talk, we investigate the properties of different choices of Riemannian metrics and their impacts on the structure of our shape space. Moreover, we present a shape space of piecewise-smooth shapes, which has the structure of a Riemannian product manifold. Finally, we investigate the optimization of multiple shapes.

Geometry-based Solutions to Multivariate Minimization Problems

Hütter, Sebastian; Halle, Thorsten
Otto von Guericke University Magdeburg

15:20

For the calculation of phase diagrams from thermodynamic data, a constrained minimization problem over a linear combination of several non-linear free enthalpy functions has to be solved. Conventional methods work well if these functions are continuous and differentiable in all variables. In a novel calculation approach, the basic thermodynamic data is available only on discrete points in parameter space, making a different solution method necessary. Such a method is developed from analytic geometry and its general applicability to phase equilibria is shown. Possible special cases occurring in the calculation of phase diagrams from ab-initio free energies are discussed. The resulting solutions are then examined with regard to consistent identification of the phases in equilibrium by application of a graph coloring scheme with matching of subsequent executions to the same coloring, regardless of numerical differences.

A set-valued stochastic approximation analysis of two-timescale actor-critic reinforcement learning with non-linear function approximation and clipped gradients

Redder, Adrian; Kayacan, Erdal
Paderborn University

15:40

Actor-Critic (AC) is a fundamental paradigm for the design of data-driven adaptive decision-making and control approaches. AC improves an actor sequentially based on the evaluation of a critic. Simultaneously with the actor, the critic is updated to accurately evaluate the actor's control decisions. Therefore, the paradigm results in two coupled iterations deeply rooted in reinforcement learning and stochastic approximation (SA). However, huge gaps exist between AC's practically observed properties and theoretically desirable properties, such as stability and convergence. The core challenge lies in non-linear function approximators, such as neural networks, for approximating the actor and the critic. Historically, AC algorithms have been studied as two-timescale algorithms, where the critic is updated on a faster time scale, i.e., with an asymptotically larger stepsize than the actor, such that the critic iteration sees the actor as asymptotically stationary; in contrast, the actor sees the critic as asymptotically equilibrated. The challenge for two timescale analyses in the presence of non-linear function approximation is that the SA solution is generally not unique, which leads to asymptotically set-valued dynamics for the coupled AC iteration.

As a first step towards a better understanding of practical implementations of AC, we present an analysis of AC reinforcement learning with non-linear function approximation and clipped gradients studied as a two-timescale stochastic approximation algorithm with set-valued dynamics. Specifically, we study deterministic policy gradient algorithms for compact state-action spaces, where non-linear function approximators represent the actor and the action-value function (critic). Both the actor and

the critic are updated using clipped gradient information to ensure the stability of the coupled AC iterations. Our convergence analysis shows that the critic iteration converges to a stationary point of the average clipped critic gradient evaluated at the obtained actor limit. The averaging is taken with respect to the limit of a continuous time measure process that captures the encountered experience of the AC iteration in the optimization environment. For the actor, we show that the actor parameters converge to a stationary point of the averaged actor gradient taken with respect to a point in the convex-hull over the critic parametrizations that obtain zero critic gradient for the actor limit. This property leads to better generalizability beyond the state-space encountered during training for the obtained actor policy compared to a single-timescale AC implementation. This explains why, in practical implementations, the critic stepsize is usually chosen at least 1-2 magnitudes larger than the actor stepsize.

S16.05: Nonsmooth Problems II

Date: March 20, 2024 16:30–18:30
Room: G22/110
Chair(s): Herberg, Evelyn
Kahle, Christian

Using a Quadratic Constrained Active Signature Method to Solve Nonsmooth Retail Portfolio Maximization Problems

Kreimeier, Timo; Kannan, Aswin; Walther, Andrea 16:30
Humboldt-Universität zu Berlin

In this talk, we present an optimization algorithm for solving so-called Abs-quadratic constrained optimization problems and apply it to nonsmooth retail portfolio problems.

Abs-quadratic functions comprise all functions that have a piecewise quadratic structure and can be rewritten using the absolute value with a linear argument. Using this structure the feasible space can be divided into polyhedra. Optimality criteria are then used to solve a suitable sequence of subproblems on these polyhedra.

For the resulting algorithm, which we call Quadratic Constrained Active Signature Method, we prove finite convergence. We also present its application to retail portfolio maximization problems, which consist of two optimization problems solved in sequence. The first task is an estimation problem, where the underlying objective is to predict the coefficients of demand elasticity with respect to product prices. The second one is a dynamic revenue maximization problem that takes these coefficients as inputs. The obtained numerical results are discussed.

Towards a practical conjugate gradients method for semismooth problems

Bergmann, Enrico; Bethke, Franz; Walther, Andrea 16:50
Humboldt-Universität zu Berlin

For an extensive class of large scale nonsmooth optimization problems proper algorithmic differentiation tools can be used to compute generalized gradients. Hence, these tools thereby provide the first order oracle that is used to drive first order optimization algorithms. More specifically, for any direction, it is possible to computed generalized gradients that achieve the same relation to the directional derivative as their regular counterparts in the smooth case. The conceptual semismooth conjugate gradient (SSCG) method uses a convex combination of two of these directionally active gradients that matches the orthogonality condition of an exact line search in the smooth case. This orthogonality is then used in a shortest residual update of the search direction that drives the analysis of the method. However, the caveat of the conceptual SSCG method is, that it requires an exact line search in nonsmooth case as well.

After a recap of the aforementioned concepts the talk discusses how this requirement can be softened using suitable line search termination conditions. Specifically two conditions are taken into account, one for that case that the optimal step size results in a point close to a nondifferentiablity and one Wolfe-like-condition for step sizes that result in a point were the objective is smooth or almost smooth.

The talk then presents possible ideas in recovering the theoretical results of the conceptual SSCG method, if in the analysis of the outer algorithm the epsilon-Goldstein differential is used instead of the Clark differential.
Preliminary numerical tests that showcase the effectiveness of the obtained method will be presented towards the end of the talk.

About Solving Complementarity Problems by Combining SCIP with a Piecewise Linear Solver

Kreimeier, Timo (1); Pfetsch, Marc (2); Schmidt, Adrian (1); Walther, Andrea (1)

1: Humboldt-Universität zu Berlin
2: TU Darmstadt

17:10

In this talk, we consider finding global minima for constrained piecewise linear optimization problems. One particular structure that fits this setting is complementarity constraints. Because they can be expressed in terms of the absolute value function, they can also be represented in the so-called abs-linear form - a matrix-vector representation. This allows us to handle them with the Constrained Active Signature Method, a solver for constrained piecewise linear optimization problems.

We present the incorporation of this algorithm into a global solver like SCIP to determine not only local minima, but also global minima. Especially, we investigate Phase 1 for linear programs with complementarity constraints and the warm start capabilities.

Towards the end of the talk, first numerical results will be presented for different classes of problems, such as bilevel problems.

S17: Applied and numerical linear algebra

Organizer(s): Lund, Kathryn *(Max Planck Institute for Dynamics of Complex Technical Systems)*
Palitta, Davide *(Alma Mater Studiorum, Università di Bologna)*

S17.01: Applied and Numerical Linear Algebra

Date: March 20, 2024 16:30–18:30
Room: G22/208
Chair(s): Lund, Kathryn

Numerical linear algebra for data assimilation

Tabeart, Jemima M. (1); Palitta, Davide (2); Pearson, John W. (3)
1: Eindhoven University of Technology
2: University of Bologna, Italy
3: University of Edinburgh

16:30

The quality of a weather forecast is strongly determined by the accuracy of the initial condition. Data assimilation methods allow us to combine prior forecast information with new measurements in order to obtain the best estimate of the true initial condition. However, many of these approaches require the solution of an enormous least-squares problem. In this talk I will discuss some mathematical and computational challenges associated with data assimilation for numerical weather prediction, and show how structure-exploiting numerical linear algebra approaches can lead to theoretical and computational improvements. In particular I will show how re-writing the primal form of the weak-constraint 4D-Var problem as a saddle point formulation reveals the underlying block structure and hence admits a much richer class of preconditioners.

Balanced Truncation using Noisy Gramians for Bayesian Inverse Problems with Quadratic Nonlinearity

Freitag, Melina A. (1); König, Josie (1); Qian, Elizabeth (2)
1: University of Potsdam
2: Georgia Institute of Technology, USA

17:10

The posterior distribution for nonlinear Bayesian inverse problems often has to be made accessible by sampling and requires many simulations of the forward model, which is very costly in high dimensions. This can be remedied by a reduced model that captures the important dynamics. Balanced truncation methods from systems theory are a useful tool for such problems. In this work, we introduce new noisy Gramians for quadratic Bayesian inverse problems that allow model reduction by balanced truncation. The numerical linear algebra methods used are presented, and the limitations of this method, especially with respect to the stability radius, are discussed.

Low-Rank Multi-Patch IGA

Riemer, Tom-Christian (1); Bünger, Alexandra (2); Stoll, Martin (1)
1: TU Chemnitz
2: University of British Columbia, Canada

17:30

Isogeometric analysis (IGA) has become one of the most popular methods for the discretization of PDEs on complex domains, which arise in various applications of science and engineering. Thereby, it is often required to describe the computational domain of a complex geometry as multiple patches, where each patch is given by a tensor product B-spline parametrization and two such patches of a geometry are connected by an interface. In this setup the crucial challenge lies in the solution of the discretized equations of a PDE problem, for which the discretization results in a system of large mass and stiffness tensors, which are typically very costly to assemble and may become infeasible to treat with conventional methods due to its size. Furthermore, the continuity on the interfaces of the approximation must always be guaranteed. In this talk we illustrate that low-rank methods based on the Tensor-Train (TT) format in combination with the Block-AMEn (alternating minimal energy) iterative solver, where the discretization of the PDE is formulated as a low-rank structure with Kronecker

products between its individual spatial dimensions, can be generalised for multi-patch geometries by integrating an isogeometric tearing and interconnecting (IETI) approach, by extending the linear system with constraint tensors and Lagrange multipliers, which enforce continuity on the respective interfaces. Numerical tests implemented in MATLAB using the GeoPDEs toolbox confirm this theory.

Real-world datasets ideality for photometric stereo under unknown lighting

Crabu, Elisa (1); Pes, Federica (2); Rodriguez, Giuseppe (1); Tanda, Giuseppa (3)
1: University of Cagliari
2: University of Pisa
3: CeSim – Centro Studi "Identità e Memoria", Italy

17:50

Photometric stereo is a computer vision technique for reconstructing the shape of a 3D object starting from 2D pictures. The model requires that the object surface is Lambertian and that the light sources are positioned at infinite distance from it. In real datasets these assumptions are not fully verified. Indeed, in real scenarios it is often impossible to accurately measure the relative position between the light sources and the target. This situation is common in archaeological applications, which is the topic of our studies. The Hayakawa procedure gives an estimation of lights positioning directly from the images, but in some cases it breaks down because some of the dataset images deviate from ideality. In order to understand which images from a given dataset should be selected to produce a better reconstruction, we introduce and discuss two measures of data ideality. We finally investigate the performance of these measures on synthetic experimental datasets.

On the injectivity radius of the Stiefel manifold

Stoye, Jakob (1); Zimmermann, Ralf (2)
1: TU Braunschweig
2: University of Southern Denmark

18:10

The Stiefel manifold *St(n,p)* is the set of rectangular matrices of dimension *n*-by-*p* with orthonormal columns. Stiefel manifolds feature in applications such as computer vision, medical image analysis and parametric model reduction. The geodesics on the Stiefel manifold starting from $U \in St(n,p)$ are given by the Stiefel exponential $Exp_U(t\Delta)$ at U for a normalized tangent direction $\Delta \in T_U St(n,p)$. Geodesics are candidates for shortest paths and are unique shortest paths when the starting velocity stays within the so-called injectivity radius. The same condition ensures that the Stiefel exponential at U and thus the Riemannian normal coordinates at that location are invertible. In this case, we are able to calculate the shortest path between two given points. Solving the geodesic endpoint problem is important, e.g., for interpolation tasks and for computing Riemannian centers of mass.

Using a standard curvature argument, Rentmeesters [1] has shown that the injectivity radius of the Stiefel manifold is bounded by $\sqrt{4/5}\pi$. It is an open question, whether this bound is sharp. With the definition of the injectivity radius via cut points of geodesics in [2], we gain access to the investigation of the injectivity radius by investigating geodesics. Since the theoretical analysis of geodesics for cut points and especially conjugate points as a type of cut points is difficult, we investigate the question of the sharpness of the bound by means of numerical experiments. For a better understanding of cut points, we present an example of a conjugate point and construct an explicit cut point in a specific setting.

References

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[2] Manfredo P. do Carmo and Francis Flaherty. Riemannian Geometry. Birkhäuser Boston, MA, second edition, 1993.

S17.02: Applied and Numerical Linear Algebra

Date: March 21, 2024 08:30–10:30
Room: G22/208
Chair(s): Lund, Kathryn

Riemannian optimization on the symplectic Stiefel manifold

Gao, Bin (1); Son, Nguyen Thanh (2); Stykel, Tatjana (3)
1: Chinese Academy of Sciences, China
2: Thai Nguyen University of Sciences, Vietnam
3: University of Augsburg

08:30

Optimization problems on the symplectic Stiefel manifold find applications in various areas such as quantum mechanics, model order reduction and data analysis. By introducing a new family of Riemannian metrics on the symplectic Stiefel manifold that includes the canonical-like and Euclidean metric as a special case, we establish the closed-form expressions for geometric ingredients including orthogonal projections, vector transports, Riemannian gradient and Hessian of matrix functions. Further, we present different Riemannian optimization algorithms such as gradient descent, conjugate gradient and Newton's methods, and discuss their convergence. Numerical experiments for several optimization problems illustrate the efficiency of these methods.

Optimization of Approximate Maps for Linear Systems Arising in Discretized PDEs

Islam, Rishad; Carr, Arielle; Jacobs, Colin
Lehigh University, USA

08:50

Generally, discretization of partial differential equations (PDEs) creates a sequence of linear systems $A_k\, x_k = b_k$, k = 1, 2, ..., N with well-known and structured sparsity patterns. When approximately solving these linear systems using iterative solvers, preconditioners are often necessary to achieve fast convergence. For closely related systems, we can use preconditioner updates instead of computing a preconditioner for each system from scratch. One such preconditioner update is the sparse approximate map (SAM) (Carr et al., 2021), which is based on the sparse approximate inverse preconditioner using a least squares approximation. A SAM then acts as a map from one matrix in the sequence to another nearby one for which we have an effective preconditioner. To efficiently compute an effective SAM update (i.e., one that facilitates fast convergence of the iterative solver), we seek to compute an optimal sparsity pattern. In this talk, we examine several sparsity patterns for computing the SAM update in an effort to characterize optimal or near-optimal sparsity patterns for linear systems arising from discretized PDEs. The allowable number of nonzeros in the sparsity pattern should strike a balance between the accuracy of the map and the cost to apply it in the iterative solver. We can show that the sparsity pattern of the exact map is a subset of the sparsity pattern of the transitive closure of a graph representation of A_k, $G(A_k)$. As a result, we focus our attention on level 1 and level 2 neighbors of $G(A_k)$ based on analysis in (Chow, 2000), as well as an element-wise analysis on the difference matrix between two nearby matrices e.g., k^{th} and $(k\text{-}1)^{st}$ matrix. We modify the current implementation of the SAM update to account for the changing sparsity pattern and matrix entries of A_k in the sequence. Additionally, we extend the existing analysis to show that if our sequence of linear systems satisfies simple subset assumptions, we can characterize properties of the residual matrix emitted from the approximate map.

Preconditioning and deflation in the action of the matrix sign function with an application to Lattice QCD

Ramirez-Hidalgo, Gustavo; Finkenrath, Jacob
University of Wuppertal

09:10

In a recent work [Burke, Frommer, R-H, Soodhalter; 2022], an algorithm for deflating+recycling in a sequence of applications of a function of a matrix times a vector, i.e. $f(A_i)b_i$, i=1,...,N with N the length of the sequence, was developed. The method shows an acceleration in convergence, with a limitation of not being clear how to restart the underlying Arnoldi process. In another work [Frommer, R-H, Schweitzer, Tsolakis; in preparation], polynomial preconditioning for $f(A)b$ is proposed, which accelerates convergence hence reducing the total number of dot products, and opening to the possibility of not having to do restarts. In this talk we explore the combination of both methods. The polynomial spreads the low modes, making it easier for the deflation+recycling method to build the preconditioned low modes via the augmented subspace. Also, the polynomial allows us to overcome

the limitation of the deflation+recycling method in the sense of restarts. Furthermore, we study how information from the construction of the polynomial can be used to help in the construction of the recycling subspace, and conversely, we try to use the recycling subspace information to build a better polynomial to precondition the next $f(A_i)b_i$ application in the sequence. The matrix function we use is $f(A) = sign(A)$, where $sign(A) = A(A^2)^{-1/2}$, with A being directly related to the Wilson-Dirac operator at nonzero chemical potential from Lattice Quantum Chromodynamics.

Recycling of Krylov subspaces in the simulation of nonlinear dynamic systems
Stellmach, Laurenz; Nitzschke, Steffen; Woschke, Elmar
Otto von Guericke University Magdeburg
09:30

In the transient simulation of rotating systems with aero- or hydrodynamically operating journal bearings, non-linear systems of equations must be solved repeatedly to determine the bearing pressure. Usually, a Newton-Raphson method is used for this purpose, whereby a series of linear systems of equations occurs at each time step. The resulting system matrices are always sparse and show an identical filling structure, but with varying entries. Up to now, these systems of equations have been solved iteratively using established methods (GMRES, BiCG, BiCGStab). Since the entries in the system matrix change only slowly over time, it makes sense to pick up information from a previous solution attempt and reuse it for the new solution in the new time step in order to accelerate convergence and minimize the computational effort. Such methods can be found in the recycling Krylov method, where a given subspace is used to increase the convergence speed. In this paper, an rBiCGstab method is applied, using either a block GMRES method or a modal analysis to generate the subspace. The paper discusses the implementation of these methods within the time integration described above, with an evaluation in terms of convergence and necessary computing time.

Struture preserving approximations to Cayley transforms
Frommer, Andreas; Diab, Malak; Kahl, Karsten
University of Wuppertal
09:50

The Calyely transform arises in particular in time-stepping of ODEs and DAEs using the implicit midpoint rule. For systems with dissipation, and in particular for port-Hamiltonian systems, structure preservation such as conservation of energy or stabilty / conservation of dissipation are important.

In this talk we show that the "energy-orthogonal" matrix function Arnoldi approximation to the Cayley transform preserves these structural properties for each iterate, i.e. not only in the limit. This also holds if the energy-norm is actually only a seminorm, as it might be the case with DAEs. We analyze numerical properties and modifications of the Arnoldi process in particular for the DAE case.

Reorthogonalized Pythagorean variants of block classical Gram Schmidt
Carson, Erin (1); Lund, Kathryn (2); Oktay, Eda (1)
1: Charles University, Czech Republic
2: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
10:10

The computation of Krylov subspace methods (KSMs) and orthogonalization procedures requires sparse matrix-vector products (SpMV) and inner products in each iteration. These operations are also called synchronization points, due to the data movement between levels of cache on a node or the message-passing operations necessary in distributed computing, and they cause KSMs to be communication bound. To reduce communication costs, communication-avoiding Krylov methods can be employed, which make use of the sparse matrix powers kernel and a batched or “block" orthogonalization of basis vectors.

Block Classical Gram-Schmidt (BCGS) is a common choice for the block orthogonalization process, as it requires only two synchronization points in addition to an SpMV per iteration. However, BCGS is known to have a high loss of orthogonality, which can contribute to instability and inaccurate solutions in the overall KSM. To balance performance and stability, a so-called “Pythagorean" variant of BCGS

was introduced in [E. Carson, K. Lund, & M. Rozložník. *The stability of block variants of classical Gram-Schmidt*. *SIAM J. Matrix Anal. Appl.* 42(3), pp. 1365–1380, 2021] that guarantees an $O(\varepsilon)\kappa^2(X)$ bound on the loss of orthogonality as long as $O(\varepsilon)\kappa^2(X) < 1$, where ε denotes the working precision.

We introduce two reorthogonalized Pythagorean BCGS variants, each with the same number of synchronization points as BCGS, to improve stability. We show how reorthogonalization can restore an $O(\varepsilon)$ bound on the loss of orthogonality both in theory and in practice.

S17.03: Applied and Numerical Linear Algebra

Date: March 21, 2024 14:00–16:00
Room: G22/208
Chair(s): Palitta, Davide

Sketched and truncated Krylov methods for core linear algebra problems

Schweitzer, Marcel 14:00
University of Wuppertal

Randomized methods based on the sketch-and-solve paradigm have originally been developed for applications with rather crude accuracy demands. Yet, by combining them with (polynomial) Krylov subspace methods, they have recently been successfully applied to linear algebra problems with high accuracy requirements, like solving linear systems and matrix equations or approximating matrix functions.
The key idea in many of these algorithms is combining a truncated orthogonalization with an oblivious subspace embedding that mitigates the negative effects of lack of orthogonality and this way (almost) restores convergence properties of the full method, while significantly reducing cost, storage demands and communication.
This comes at a cost, though: Implementation becomes more cumbersome (particularly for more involved problems like matrix equations) and hyperparameters like the embedding dimension are introduced. At the same time, an analysis of the methods also becomes highly nontrivial, as sketching might alter the spectral properties of the problem significantly, to a point where one would often not expect the methods to work at all. Yet, almost magically, they still perform very well for many problems of interest.
In this talk, we give an overview of recent advances both on the algorithmic front and concerning convergence analysis and theoretical guarantees, in order to explain why the great practical performance might be less magical than it seems at first sight.

A new rational Krylov subspace based projection method for solving large-scale algebraic Riccati equations via low-rank approximations

Faßbender, Heike 14:40
TU Braunschweig

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 though 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 X_i stored in low-rank factored form. That is, the Hermitian low-rank approximations X_j to X are 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 belongs to the rational Krylov subspace based methods as it is based on projecting the CARE onto a certain block rational Krylov subspace spanned by blocks of the form $(A^H+ \sigma_jI)C^H$ for shifts σ_j. The resulting projected Riccati equation is then solved for Y_j. The considered projections do

not need to be orthogonal and are built from the matrices appearing in the block rational Arnoldi decomposition associated to the block rational Krylov subspace considered. The approximations X_j as well as the residual norm $||R(X_j)||_F$ can be computed fast and efficiently. The resulting method generates an approximate solution X_j which may be indefinite due to rounding errors. We suggest to truncate the unwanted eigenvalues which leads to an approximation of even lower rank. We prove that this truncated approximate solution can be interpreted as the solution of the Riccati residual projected to a subspace of the block rational Krylov subspace considered. This gives us a way to efficiently evaluate the norm of the resulting residual. Numerical examples will be presented.

Extreme solutions of algebraic Riccati inequalities
Mehrmann, Volker (1); Xu, Hongguo (2)
1: TU Berlin
2: University of Kansas, USA
15:00

The characterization of the solution set for a class of algebraic Riccati inequalities is studied. This class arises in the passivity analysis of linear time invariant control systems. Eigenvalue perturbation theory for the Hamiltonian matrix associated with the Riccati inequality is used to analyze the extremal points of the solution set.

Low-rank solution of restricted discrete-time Gramians
Kürschner, Patrick
Leipzig University of Applied Sciences (HTWK Leipzig)
15:20

We consider the approximate computation of Gramians of large-scale linear discrete-time state-space systems. In particular, the focus will be on the Gramians which arise in time- and frequency-limited balanced truncation model order reduction.

While there are many results for the continuous-time situation, the discrete-time scenario is usually considered to a much lesser extent.

The Gramians are solutions of discrete-time Lyapunov matrix equations (also called Stein matrix equations) which, if the reduction is restricted to finite time or frequency intervals, also incorporate matrix functions. In the present situation, these functions come in the form of matrix powers or matrix logarithms.

We discuss the efficient numerical handling of these matrix function as well as the computation of low-rank Gramian approximation by rational Krylov subspace and related iterative methods.

S17.04: Applied and Numerical Linear Algebra
Date: March 22, 2024 08:30–10:30
Room: G22/208
Chair(s): Palitta, Davide

A new fast numerical method for the generalized Rosen-Zener model and its application to matrix exponential approximation
Bonhomme, Christian (2); Van Buggenhout, Niel (1); Pozza, Stefano (1); Zahid, Shazma (1)
1: Charles University, Czech Republic
2: Sorbonne Université
08:30

In quantum mechanics, the Rosen-Zener model represents a two-level quantum system. Its generalization to multiple degenerate sets of states leads to a larger non-autonomous linear system of ordinary differential equations (ODEs). We propose a new method for computing the solution operator of this system of ODEs. This new method is based on a recently introduced expression of the solution in terms of an infinite matrix equation, which can be efficiently approximated by combining truncation, fixed point iterations, and low-rank approximation. This expression is possible thanks to the so-called $*$-product approach for linear ODEs. In the numerical experiments, the new method's computing time scales linearly with the model's size. We provide a first partial explanation of this

linear behavior. When the system is autonomous, this approach also produces a new method for computing the matrix exponential.

Adaptive rational Krylov methods for exponential Runge–Kutta integrators

Bergermann, Kai; Stoll, Martin
TU Chemnitz

08:50

We consider the solution of large stiff systems of ordinary differential equations with explicit exponential Runge–Kutta integrators. These problems arise from semi-discretized semi-linear parabolic partial differential equations on continuous domains or on inherently discrete graph domains. A series of results reduces the requirement of computing linear combinations of φ-functions in exponential integrators to the approximation of the action of a smaller number of matrix exponentials on certain vectors. State-of-the-art computational methods use polynomial Krylov subspaces of adaptive size for this task. They have the drawback that the required number of Krylov subspace iterations to obtain a desired tolerance increase drastically with the spectral radius of the discrete linear differential operator, e.g., the problem size. We present an approach that leverages rational Krylov subspace methods promising superior approximation qualities. We prove a novel a-posteriori error estimate of rational Krylov approximations to the action of the matrix exponential on vectors for single time points, which allows for an adaptive approach similar to existing polynomial Krylov techniques. We discuss pole selection and the efficient solution of the arising sequences of shifted linear systems by direct and preconditioned iterative solvers. Numerical experiments show that our method outperforms the state of the art for sufficiently large spectral radii of the discrete linear differential operators. The key to this are approximately constant numbers of rational Krylov iterations, which enable a near-linear scaling of the runtime with respect to the problem size.

Mixed-precision Paterson–Stockmeyer method for evaluating matrix polynomials

Liu, Xiaobo
University of Manchester, UK

09:10

The Paterson–Stockmeyer method is an evaluation scheme for matrix polynomials with scalar coefficients that arise in many state-of-the-art algorithms based on polynomial or rational approximants, for example, those for computing transcendental matrix functions. We derive a mixed-precision version of the Paterson–Stockmeyer method that can be faster than its fixed-precision counterpart while delivering the same level of accuracy.

The Fréchet derivative of the tensor t-function

Lund, Kathryn (1); Schweitzer, Marcel (2)
1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: University of Wuppertal

09:50

The *tensor t-function*, a formalism that generalizes the well-known concept of matrix functions to third-order tensors, is introduced in Lund (Numer Linear Algebra Appl 27(3):e2288). In this work, we investigate properties of the Fréchet derivative of the tensor t-function and derive algorithms for its efficient numerical computation. Applications in condition number estimation and nuclear norm minimization are explored. Numerical experiments implemented by the t-Frechet toolbox hosted at https://gitlab.com/katlund/t-frechet illustrate properties of the t-function Fréchet derivative, as well as the efficiency and accuracy of the proposed algorithms.

S18: Numerical methods for differential equations

Organizer(s): Wieners, Christian *(Karlsruher Institut für Technologie)*
Freese, Philip *(Hamburg University of Technology)*

S18.01: Discontinuous Galerkin and Software

Date: March 19, 2024 08:30–10:30
Room: G22/020
Chair(s): Wieners, Christian

Voronoi diagrams and Finite Volume methods in any dimension

Heida, Martin 08:30
Weierstrass Institute for Applied Analysis and Stochastics

We introduce HighVoronoi.jl, a package that can effectively calculate Voronoi diagrams in any dimension, for generators in general and non-general position and including (periodic) convex polytope boundaries. It also implements the Finite Volume discretization of second order PDEs in various settings.

We shortly discuss the newly developed algorithm and the underlying new mathematics and provide a few examples.

DG-type reconstructions for SBP finite difference schemes

Bach, Daniel; Gassner, Gregor J.; Rueda-Ramírez, Andrés M. 08:50
University of Cologne

Schemes with the summation by parts property are both present in a finite difference and a discontinuous Galerkin context. In a DG scheme this can be interpreted as the property that the interpolating polynomials together with the numerical integration rule chosen fulfill a discrete analogue of the integration by parts property. Because of this property one can for example prove discrete conservation for nonlinear conservation laws or entropy stability for certain SBP-DG schemes by replacing integration by parts in proofs for the analytic functions with summation by parts in the discrete case. Many proofs of this kind only rely on the fact that the discrete operator fulfills the SBP property, but not that they come from a DG ansatz. Thus they also hold for SBP-FD schemes.

The derivative matrix of the DGSEM scheme is a DG scheme using collocation of quadrature and interpolation points from the Lagrange basis polynomials, where each column is a vector of derivative values of one basis function on the interpolation points. In FD schemes however the derivative matrix is made up of the stencils used to approximate the derivative on the FD points. The derivative matrix of the DG scheme can be reinterpreted as a FD derivative matrix using a different stencil for each interpolation point. This talk examines the question if this reinterpretation can be done the other way around, meaning if there are function spaces and basis functions that reproduce the FD derivative matrix as columns of basis derivatives.

If using a DG type discretization results in the same discrete scheme. the SBP-FD schemes could be reinterpreted as a type of finite element type scheme, which means the solution is now globally defined instead of just on discrete point values. This would allow for the evaluation of the FD solution on arbitrary points and also for global error estimates of the approximation.

This talk will also examine the properties of these possible SBP-FD reconstructions, especially in regards to locality. The derivative matrices of FD operators are usually not dense contrary to the ones used in DG schemes, which suggests that possible basis function should have a local support contrary to the polynomials used in the DG ansatz.

Monolithic Convex Limiting For Legendre–Gauss–Lobatto Discontinuous Galerkin Spectral Element Methods

Rueda-Ramírez, Andrés M. (1); Bolm, Benjamin (1); Kuzmin, Dmitri (2); Gassner, Gregor (1)
1: University of Cologne
2: TU Dortmund University

09:10

In this talk, we present a subcell flux correction procedure for nonlinear hyperbolic problems, the so-called Monolithic Convex Limiting (MCL). It uniquely merges a high-order baseline discretization with an invariant domain-preserving low-order scheme. This *a-priori* limiting approach operates at the node level, exploiting the stability advantages of the low-order method while retaining the superior accuracy of the high-order scheme. This allows us to run simulations for challenging setups with strong shocks, steep density gradients and vortex dominated flows, which we will present in this talk. Our innovation extends the original monolithic convex limiting concept to a high-order Discontinuous Galerkin discretization on Legendre–Gauss–Lobatto nodes, which greatly simplifies the design of invariant domain-preserving high-resolution schemes. One of the distinguishing features of our methodology is its adaptability, which allows for multiple options of limiting. This flexibility includes the use of different proportions of the low-order scheme for different conservative variables, thereby avoiding unnecessary limiting and the consequent loss of accuracy. The methods have been implemented and tested within Trixi.jl – an advanced high-order numerical simulation framework for conservation laws – using the programming language Julia. DOI: http://dx.doi.org/10.48550/arXiv.2303.00374

Numerical Solution of Ultra-Relativistic Euler Equations using Discontinuous Galerkin Finite Element Method

Mairaj, Muhammad
COMSATS University Islamabad, Pakistan

09:30

In this work, numerical solutions of ultra-relativistic hydrodynamics equations (URHD) have been studied and analyzed. Relativistic hydrodynamics (RH) has a key role to play in areas like cosmology, high-energy astrophysics, and nuclear physics. Taking into account the special relativity, the model problem explains the dynamics of the perfect compressible fluid. These equations are more complicated than non-relativistic ones because of their non-linearity and complex nature as well. It is hoped that the numerical schemes will produce precise, adequate, and robust approximate solutions. The Discontinuous Galerkin Finite Element Method (DG-FEM) is applied in this study to solve the URHD model. The proposed scheme is high-order accurate, stable, and capable of dealing with complex geometries.

deal.t: An implementation of T-splines within the `deal.II` framework

Beuchler, Sven; Hiniborch, Robin; Morgenstern, Philipp
Leibniz University Hannover

09:50

Modelling domains to solve partial differential equations (PDEs) with the classical finite element method (FEM) will usually lead to discretization errors unless special measures are taken. Thus, isogeometric analysis (IGA) introduced the use of the modelling B-spline basis functions from the CAx-modelling to remove these errors. However, local h-refinement, i.e. knot insertion, with B-Splines is problematic. This is due to the definition of B-Spline basis functions on a tensor-product mesh, which allows knot insertion only on a global scale. Hence, further techniques have been introduced to adaptively refine meshes using error estimation, e.g. LR B-Splines, hierarchical B-Splines, and T-Splines. A major benefit for T-Splines in contrast to other techniques is the guaranteed locally linear independency of basis functions through a geometric condition.
On the other hand, Spline basis functions are defined to span multiple cells of a triangulation, i.e. one basis function has support on more than one cell. This leads to a varying amount of basis functions, i.e. degrees of freedom, for each cell. While this is no problem for IGA-FEM implementations, e.g. G+Smo, it needs to be solved for a standard FEM implementation, e.g. deal.II. The solution for T-Splines is given by the geometric condition for linear independency, which yields another refinement

step to ensure this.
In this talk, we present deal.t, an isogeometric framework to solve PDEs with no discretization errors through T-Splines. We give a short introduction to T-Splines and the geometric condition necessary for locally linear independent T-Splines in two and three dimensions. As spline values on each cell are evaluated through Bézier extraction as a linear combination of Bernstein polynomials, we will give the idea of Bézier extraction for T-Splines. From this, we further discuss the different meshing classes involved with T-Splines and explain in detail the idea behind the implementation of T-Splines within deal.t. Before we finish the talk by some examples given in two and three spatial dimensions, we will give a short code-snippet on how to use deal.t in contrast to its base deal.ii.

TrixiParticles.jl: an accessible numerical framework for particle-based simulations in Julia
Faulhaber, Erik (1); Neher, Niklas (2); Berger, Sven (3); Schlottke-Lakemper, Michael (4); Gassner, Gregor (1)
1: University of Cologne
2: HLRS
3: Helmholtz-Zentrum Hereon
4: RWTH Aachen University/HLRS
10:10

TrixiParticles.jl is a numerical simulation framework for particle-based multi-physics simulations implemented in Julia. Our primary goal is to provide a user-friendly open-source package, accessible also to those unfamiliar with particle-based methods. Therefore, TrixiParticles.jl is designed with easy extensibility in mind, allowing researchers to quickly experiment with new models or methods without having to study and modify large parts of the code. We further try to achieve the highest possible performance without compromising readability and ease-of-use. This enables users not only to quickly prototype new ideas, but also to efficiently scale up to medium-sized simulations.
In this talk, we will give a short introduction to the Smoothed Particle Hydrodynamics (SPH) method and present some simulation results. We will then demonstrate how to extend TrixiParticles.jl by adding new models.

S18.02: Nonlinear and port-Hamiltonian systems

Date: March 19, 2024 16:30–18:30
Room: G22/020
Chair(s): Freese, Philip

Energy-adaptive and Riemannian Newton methods for Problems of Kohn-Sham Type
Altmann, Robert (1); Peterseim, Daniel (2); Stykel, Tatjana (2)
1: Otto von Guericke University Magdeburg
2: University of Augsburg
16:30

We consider the numerical solution of nonlinear eigenvector problems arising in computational physics and chemistry such as the Kohn-Sham model. Formulated as energy minimization problem on the infinite-dimensional Stiefel manifold, Riemannian optimization techniques can be used for the construction of numerical schemes. In this talk, we present a Riemannian gradient descent method (induced by an energy-adaptive metric) as well as the Riemannian Newton method. Numerical experiments will be shown to illustrate the performance of these methods.

The least-squares method in the theory of nonlinear periodic boundary value problems with concentrated delay
Benner, Peter (1); Chuiko, Sergey (1,2); Chuiko, Viktor (3)
1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: Donbass State Pedagogical University
3: Taras Shevchenko National University of Kyiv
16:50

Among numerous studies of functional-differential equations, research on periodic boundary value problems for differential equations with concentrated delay holds a special place. This is primarily

due to the wide application of periodic boundary value problems for differential equations with concentrated delay in physics, chemistry, economics, biology and mechanics.

The construction of solutions for nonlinear boundary value problems using the method of simple iterations and the least-squares method is significantly complicated by the computation of derivatives of the nonlinearities. Given this, simplifying the computation of nonlinear derivatives and the potential to find solutions for nonlinear boundary value problems, including periodic boundary value problems, in the form of elementary functions can be achieved using the Adomian decomposition method. Additionally, the use of the Adomian decomposition method significantly simplifies the proof of convergence of iterative schemes for constructing solutions to nonlinear boundary value problems.

By applying the hybrid technique based on the least-squares method and the Adomian decomposition method, we have derived the necessary and sufficient conditions for the existence of solutions to the weakly nonlinear periodic boundary value problem for a system of differential equations with concentrated delay in the critical and noncritical case. As examples of application of the constructed iterative scheme, we obtain approximations to the solutions of a periodic boundary value problem for the mathematical model of non-isothermal chemical reactions. To check the accuracy of the proposed approximations, we evaluate discrepancies in the original equation with concentrated delay.

Adomian decomposition method for nonlinear boundary-value problems unsolved with respect to the derivative

Benner, Peter (1); Chuiko, Sergey (1,2); Nesmelova, Olga (3) 17:10

1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: Donbas State Pedagogical University, Ukraine
3: Institute of Mathematics of the National Academy of Sciences of Ukraine

We have found constructive necessary and sufficient conditions for solvability and a scheme for constructing solutions for a nonlinear boundary-value problem unsolved with respect to the derivative. On the basis of the Adomian decomposition method, convergent iteration schemes computing approximations to solutions of a nonlinear boundary-value problem unsolved with respect to the derivative are constructed.

The relevance of studying the nonlinear boundary-value problem, unsolved with respect to the derivative, is related to the fact that the study of the traditional problem, which is solved with respect to the derivative, is sometimes complicated, for example, in the case of nonlinearities that are not integrable in elementary functions. An example of such a situation will be given in our report. An example of such a situation can also be an autonomous boundary-value problem unsolved with respect to the derivative, in particular, it can be the periodic problem for the Lotka-Voltaire equation.

At the same time, when constructing solutions to the nonlinear boundary-value problems with the traditional iteration scheme the problem of the impossibility of finding solutions in elementary functions once again arises, which, in turn, leads to large errors in the solutions of nonlinear boundary-value problems. In addition, the construction of solutions of nonlinear boundary-value problems, for example, with using the method of simple iterations is significantly complicated by the calculation of derivative nonlinearities. We achieve the acceleration of the convergence of iterative schemes by calculating the derivatives of nonlinearities at each step. Given the above, we have simplified the computation of derivatives of nonlinearities and the possibility of finding solutions of nonlinear boundary-value problems, in particular periodic boundary-value problems, in elementary functions using the Adomian decomposition method. In this case, the use of the Adomian decomposition method significantly simplified the proof of convergence of iteration schemes for constructing solutions of nonlinear boundary-value problems.

As examples of the application of the constructed iterative scheme, approximations to the solutions of a periodic boundary-value problem for a Rayleigh-type equation unsolved with respect to the derivative are found, including the case of a periodic problem for the equation that determines the motion of a satellite in an elliptical orbit.

Higher-order operator splitting methods for port-Hamiltonian systems
Mönch, Marius; Marheineke, Nicole
Trier University
17:30

The lecture deals with numerical methods for solving port-Hamiltonian systems. The focus is on operator splitting methods. The aim is to derive high-order methods that preserve the port-Hamiltonian properties. Splitting methods with an order of three and higher have negative step sizes. As a result, the dissipation inequality is no longer preserved. Remedy create force-gradient methods. With the help of force-gradient terms, it is possible to construct fourth-order methods that only have positive step sizes and satisfy the dissipation inequality. Finally, the case of sixth order methods is explained.

Proper Orthogonal Decomposition for port-Hamiltonian energy networks
Ortegón Villacorte, Andrés Felipe; Hauschild, Sarah-Alexa; Marheineke, Nicole
Trier University
17:50

Proper network simulation of flows in gas or water pipes is important when we want to improve the efficiency of an energy distribution system, for example to save energy or resources. The port-Hamiltonian framework is applied to the non-isothermal Euler equations in pipe networks. Thanks to the pH modeling, mass and energy conservation are encoded in the system and appropriate coupling conditions are used in the ports and pipe connections. The Structure of the system must be preserved when new network components are added, such as consumers, producers or compressor stations. The system is discretized in space preserving the structure of the original pH system. These systems often require a fine discretization in space to converge to proper results and for this reason a strategy of model order reduction is useful to significantly reduce the computational cost of the simulation. Building on previous work, we present numerical results for large energy networks where proper orthogonal decomposition is used for model order reduction.

A posteriori estimates for a coupled piezoelectric model
Samrowski, Tatiana; Langer, Ulrich; Repin, Sergey
Zurich University of Applied Sciences
18:10

The talk is related to a coupled problem describing piezoelectric effects in an elastic body. For this problem, we deduce majorants of the distance between the exact solution and any approximation in the respective energy class of functions satisfying the boundary conditions. The majorants are fully computable and do not contain mesh dependent constants. They vanish if and only if an approximate solution coincides with the exact one and provide guaranteed upper bounds of errors in terms of the natural energy norm associated with the coupled problem studied.

S18.03: Application in mechanics

Date: March 20, 2024 08:30–09:30
Room: G22/020
Chair(s): Wieners, Christian

Solving Nonlinear Finite Element Problems in Hyperelasticity
Fesefeldt, Lina; Le Borne, Sabine; Düster, Alexander
Hamburg University of Technology
08:30

Finite element methods (FEM) for displacement problems in hyperelasticity lead to systems of nonlinear equations. These equations are usually solved with Newton's method or a related method. Based on a benchmark problem in high-order FEM, we explore traditional solution techniques for the nonlinear equation system such as step width selection and Quasi-Newton methods. We also consider algorithms specifically designed for displacement problems in nonlinear structural analysis like load step and arc-length methods. We extend traditional load step methods to a new approach exploiting the hierarchical structure of the problem and saving about 50% of computation time (vs. benchmark).

In an outlook, we discuss new developments in nonlinear preconditioning and their applicability to displacement problems in nonlinear FEM.

On recent advancements in the development of Lattice Boltzmann methods for solids

Müller, Henning (1); Panov, Justinijan (1); Schlüter, Alexander (2); Müller, Ralf (1)
1: TU Darmstadt
2: RPTU Kaiserslautern-Landau

08:50

Lattice Boltzmann (LB) methods were initially developed for fluid kinetics, but they have proven to be a quite versatile and powerful family of methods for numerical simulations in various fields of science and engineering. Rather recently, these applications have been extended to encompass solid mechanics and in particular to elastodynamics[1].

This LB method for solids[2,4] shows promising performance with fast and well scaling computations. Additionally, the domain of interest is discretized using a regular lattice, which allows for easy modeling, as well as coupling. Thus, this method could be adopted for the simulation of dynamic fracture mechanics[3].

However, stability issues arise for a range of material parameters. This is in part due to the material modeling – which is more elaborate compared to fluids – and the way stresses are incorporated.

This talk restates the LB method and its numerical modeling of constitutive laws. It is then shown how instabilities emerge. Remedies are discussed, which can widen the range of stable material parameters. The focus here lies on the collision operation, which is central to the computations of LB methods and the modeling of the underlying PDEs.

1. Escande, M., Kolluru, P. K., Cléon, L. M. & Sagaut, P. Lattice Boltzmann Method for wave propagation in elastic solids with a regular lattice: Theoretical analysis and validation. Preprint at https://doi.org/10.48550/arXiv.2009.06404 (2020).

2. Faust, E., Schlüter, A., Müller, H., Steinmetz, F. & Müller, R. Dirichlet and Neumann boundary conditions in a lattice Boltzmann method for elastodynamics. *Comput Mech* (2023) doi:10.1007/s00466-023-02369-w.

3. Müller, H., Touil, A., Schlüter, A. & Müller, R. Dynamic propagation of mode III cracks in a Lattice Boltzmann method for solids. *Arch Appl Mech* (2022) doi:10.1007/s00419-022-02306-y.

4. Schlüter, A. & Müller, H. SolidLBM - Lattice Boltzmann method for solids and fractures. (2023) doi:10.5281/ZENODO.8098747.

Higher order iterative decoupling for poroelasticity

Altmann, Robert (1); Mujahid, Abdullah (2); Unger, Benjamin (2)
1: Otto von Guericke University Magdeburg
2: University of Stuttgart

09:10

The iterative decoupling of coupled PDE problems such as poroelasticity is introduced in combination with time discretization schemes up to order 5 based on the backward differentiation formulae.
Its analysis combines techniques known from fixed-point iterations with the convergence analysis of the temporal discretization.
In this talk, we demonstrate the interplay between the error components from the operator splitting and the time discretization.

S18.04: Structure preserving methods

Date: March 20, 2024 14:00–16:00
Room: G22/020
Chair(s): Wieners, Christian

Divergence-conforming methods for transient double-diffusive flows

Bürger, Raimund (1); Khan, Arbaz (2); Méndez, Paul (3); Ruiz-Baier, Ricardo (4) 14:00

1: Universidad de Concepción, Chile
2: Indian Institute of Technology Roorkee, India
3: Escuela Politécnica Nacional, Quito, Ecuador
4: Monash University, Melbourne, Australia

The analysis of an H(div)-conforming method for a model of double-diffusive flow in porous media introduced in [Bürger, Méndez, Ruiz-Baier, SIAM J. Numer. Anal.(2019), 57:1318–1343] is extended to the time-dependent case. In addition, the efficiency and reliability of residual-based a posteriori error estimators for the steady, semi-discrete, and fully discrete problems are established. The resulting methods are applied to simulate the sedimentation of small particles in salinity-driven flows. The method consists of Brezzi–Douglas–Marini approximations for velocity and compatible piecewise discontinuous pressures, whereas Lagrangian elements are used for concentration and salinity distribution. Numerical tests confirm the properties of the proposed family of schemes and of the adaptive strategy guided by the a posteriori error indicators.

Structure preserving variational approximation of dynamic poroelasticity in first-order form

Bause, Markus; Anselmann, Mathias; Margenberg, Nils; Shamko, Pavel 14:20

Helmut Schmidt University, University of the Federal Armed Forces Hamburg

Understanding the dynamics of flow in deformable porous media is an ongoing field of research in engineering sciences, for instance in biomedical, civil and material engineering, for analyzing experimental data and designing quantitative theories based on mathematical concepts. A rigorous mathematical and numerical analysis of proposed models is still challenging due to the mixed type of the model equations, nonlinearities in constitutive relations or boundary conditions or functionals used in variational formulations of error control or optimization problems. Moreover, aspects of structure preservation of discretizations to such models have emerged as important in addition to fundamental properties like stability and convergence. Here we present a holistic framework for mathematical and numerical analysis of a coupled hyperbolic-parabolic prototype system of dynamic poroelasticity.

The coupled hyperbolic-parabolic equations are rewritten as a first-order system in space and time. Well-posedness is ensured by the abstract theory for evolutionary problems of R. Picard [R. Picard, A structural observation for linear material laws in classical mathematical physics, Math. Methods Appl. Sci., 32 (2009), pp. 1768–1803]. For discretization, tailored discontinuous Galerkin space-time finite element methods (STFEMS) maintaining stability and inheriting most of the rich structure of the continuous problem are proposed [M. Bause, S. Franz, Structure preserving discontinuous Galerkin approximation of a hyperbolic-parabolic system, Electron. Trans. Numer. Anal., submitted (2023), pp. 1–24; arXiv:2311.01264]. They allow the natural construction of higher order approximations to achieve accurate results on computationally feasible grids with a minimum of numerical costs. Error estimates are presented. Further, to realize higher order schemes that require less CPU time for achieving comparable accuracy, also solvers of optimal complexity are necessary and discussed [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., **49** (2023), Article No.: 5, pp. 1–25, DOI:10.1145/3582492; arXiv:2107.10561]. For this we propose using Krylov subspace iterations that are preconditioned by geometric multigrid methods.

The numerical performance of STFEMs and the algebraic solver for the coupled hyperbolic-parabolic system is illustrated carefully. Second-order (displacement-pressure) formulations are also encountered. A challenging three-dimensional test setting related to biomedical engineering is studied.

Structure-Preserving Numerical Methods for Nonlinear Dispersive Wave Equations
Lampert, Joshua (1); Ranocha, Hendrik (2)
1: Universität Hamburg
2: Johannes Gutenberg University Mainz
14:40

We use the general framework of summation by parts operators to construct conservative, entropy-stable and well-balanced semidiscretizations of two different nonlinear systems of dispersive shallow water equations with varying bathymetry: A variant of the coupled Benjamin-Bona-Mahony (BBM) equations and a recently proposed model by Svärd and Kalisch (2023) with enhanced dispersive behavior. Both models share the property of being conservative in terms of a nonlinear invariant. This property is preserved exactly in our novel semidiscretizations. To obtain fully-discrete entropy-stable schemes, we employ the relaxation method. We present the improved numerical properties of our schemes in various test cases.

Structure-Preserving Time Discretization of Port-Hamiltonian Systems via Discrete Gradient Pairs
Schulze, Philipp
TU Berlin
15:00

In this talk we present a structure-preserving time discretization scheme for nonlinear port-Hamiltonian systems with state-dependent mass matrix. Such systems may, for instance, arise when applying structure-preserving nonlinear model reduction techniques to high-dimensional port-Hamiltonian systems. We introduce a class of time discretization methods which is based on an extension of discrete gradient methods and ensures that the time-discrete system satisfies a power balance. Furthermore, we illustrate this property based on a numerical test case, where the time-continuous system is a nonlinear reduced-order model for an advection-diffusion problem.

Structure-preserving numerical methods for Fokker-Planck equations
Bartel, Hanna (1); Ranocha, Hendrik (2)
1: Universität Hamburg
2: Johannes Gutenberg University Mainz
15:20

A common way to numerically solve Fokker–Planck equations is the Chang–Cooper method combined with the Euler methods. However, the explicit Euler method is not unconditionally positive, and severe restrictions on the time step are needed to ensure the positivity of the scheme, and the implicit Euler method is in general non-linearly implicit. Instead, we propose to combine the Chang–Cooper method with unconditionally positive Patankar-type time integration methods. In contrast to the implicit Euler method, these methods are only linearly implicit and also higher order accurate. We describe the combined approach, analyze it, and present some relevant numerical examples demonstrating advantages compared to schemes proposed in the literature.

S18.05: Solvers

Date: March 20, 2024 16:30–18:30
Room: G22/020
Chair(s): Wieners, Christian

On a Hybridized Domain Decomposition Formulation
Schmidt, Kersten; Seibel, Timon
TU Darmstadt
16:30

In this talk, we present a mixed variational formulation on a domain decomposed into patches at the example of the Poisson problem in 2D. On each patch there are the variables (u,**q**), where **q** = **grad** u, as in the mixed problem and on the skeleton of the patches a variable μ corresponding to the trace of u is introduced. We denote this formulation as *Hybridized Domain Decomposition* (HDD), as it is inspired by Hybridized Discontinuous Galerkin methods which are FE methods with variables (u_h,$\mathbf{q}_h$) on each element and μ_h on every edge. We identify the suitable Sobolev spaces for the Hybridized

Domain Decomposition formulation and show existence and uniqueness of a solution as well as its continuous dependency on the data. To do so, the necessary norm estimates are proven and it is shown that a solution u_p of the primal formulation solves the Hybridized Domain Decomposition formulation if it holds at least that u_p is in $H^{3/2}$. For domain decomposition methods it is essential to have well-posedness on every single patch, which we show to hold for the Hybridized Domain Decomposition formulation.

To obtain a numerical method, a separate mesh on each patch is introduced that is used for an FE-discretization of the variables (u,**q**) by piecewise discontinuous polynomial functions for u and piecewise polynomial H(div)-conforming vector fields for **q**. The variable μ on the interface between the patches is approximated by continuous or discontinuous piecewise polynomial functions. The numerical method shows high order convergence in the mesh width for the h-version and even exponential convergence in the polynomial degree for the p-version for smooth solutions. For singular solutions a low order convergence rate is observed.

Matrix-free algorithms for finite element solvers in nearly incompressible hyperelasticity

Schussnig, Richard (1); Kronbichler, Martin (2)
1: University of Augsburg
2: Ruhr University Bochum

16:50

Finite element methods in solid mechanics play a fundamental role in science and engineering, where low-order approximations and related matrix-based iterative solvers and preconditioners are state-of-the-art tools for implicit analysis. Performance analysis of their implementations applied to real-world engineering applications identifies the memory bandwidth as the decisive factor. It determines the speed at which the precomputed and stored matrix entries can be loaded from memory to evaluate sparse matrix-vector products in iterative methods. Since modern computer architectures can sustain more than 100 arithmetic operations for every variable transferred from memory, so-called matrix-free approaches, which repeatedly evaluate the action of the linear operator from the underlying finite element integrals, are getting increasingly attractive [1, 2]. Such schemes were first developed for fluid-mechanics problems, but can also be fruitfully applied in solid mechanics as shown by recent advances [3, 4].

Within this work, we focus on static nearly incompressible continua considering anisotropic effects stemming from reinforcing fibers. Such models are predominantly applied in the context of tissue mechanics, and allow incorporating the exponential stiffening of collagen fibers embedded in a hyperelastic ground matrix. Applying a matrix-free approach, we combine sum-factorization and tensor-product continuous, higher-order finite elements with *hp*-multigrid to precondition iterative Krylov subspace methods. Concerning the constitutive laws, we follow the standard, purely displacement-based approach, weakly enforcing incompressibility via a penalty term.

The classical total Lagrangian form and an alternative reformulation based on integration in the spatial configuration are investigated in terms of their computational efficiency. The performance of the matrix-free operator and the geometric multigrid preconditioner is compared to a matrix-based implementation with an algebraic multigrid preconditioner in benchmark problems from biomechanics and a patient-specific model of vascular tissue. We show that matrix-free methods for finite-strain hyperelasticity are indeed promising beyond the scope of scientific benchmarks, and user adaptations of the constitutive law can be accomplished while being largely agnostic to the remaining implementation.

[1] J. Brown. Efficient nonlinear solvers for nodal high-order finite elements in 3D. *J Sci Comput*. 2010; 45(1-3): 48-63.

[2] M. Kronbichler, K. Kormann. A generic interface for parallel cell-based finite element operator application. *Comput Fluids*. 2012; 63: 135-147.

[3] D. Davydov et al., A matrix-free approach for finite-strain hyperelastic problems using geometric multigrid, *Int J Numer Methods Eng*. 2020.

[4] J. Brown et al.. Performance-Portable Solid Mechanics via Matrix-Free p-Multigrid. *ArXiv:2204.01722*. 2022. https://doi.org/10.48550/arXiv.2204.01722.

Comparison between block preconditioner and monolithic preconditioner for iterative solution of coupled multi-field problems from generalized continuum models

Alkmim, Nasser; Gamnitzer, Peter; Hofstetter, Günter 17:10
University of Innsbruck

In this work, we compare these two approaches for preconditioning the iterative solution of a coupled multi-field problem derived from a generalized continuum model. The model is aimed at simulating failure in quasi-brittle materials such as concrete and rocks and it couples microrotation and nonlocal damage fields with the displacement field. Solving large and sparse linear systems can be a challenge, especially when dealing with complex systems like multi-field problems. The success of iterative methods depends on the spectral properties of the system matrix, so careful construction of the preconditioner is crucial. A usual approach for the multi-field case involves using a block preconditioner based on factorization, which requires problem-specific approximations of the Schur complement and sub-block inverses. A popular choice for these inverse approximations is the Algebraic Multigrid Method (AMG), which has proven effective in many cases.
Another strategy is to use AMG on the entire system as a monolithic preconditioner, which treats the block structure inside the preconditioner during hierarchy construction.
Our investigations intend to demonstrate, for the proposed problem, the usefulness of treating the whole block system inside the AMG hierarchy and hence preserve the coupling aspects of the problem.

Differentiability Matching and Z-Score Normalization in Piecewise Approximated Physics Informed Neural Networks for Solving PDEs

Rout, Siddharth; Kong, William 17:30
University of British Columbia, Canada

Many partial differential equations exist that do not have exact solution; hence, numerical methods for solving PDEs are very common. However, the computational cost involved in numerical approximations can often be very high to get a stable and accurate solution which can make solving PDEs slow or imprecise if the system is large or complicated. In the field of computational mechanics, physics informed neural networks have been proposed as a new alternative to solve these equations. These neural networks are posed as approximate functions of independent variables satisfying the PDEs and are trained to minimise the residual at random points in the domain under the constraint of initial or boundary conditions. Although the technique is functionally a regression problem, this method does not require the solution points to find the fitting function. Instead, it essentially fits to the governing equations rather than physical data points. Due to the strong universal approximation capability of neural networks and generalizability, the technique has the potential to be extremely promising. To enhance optimization and scalability using parallel computation, domain decomposition as a piecewise approximation is deemed beneficial. Later models down the line focus on value matching at subdomain interfaces to penalise discontinuity. In this work, we examine the viability of differentiability matching at subdomain interfaces, a subject that has not been showcased before, along with subdomain normalization methods to improve the efficacies of existing PINN schemes. The schemes examined include extended (XPINN) and conservative (cPINN) methods to improve accuracy including various normalizations of data and applying a distributed (DPINN) scheme, which essentially adds a differentiability constraint. When analysed using standard published cases, Z-score normalization outperformed other normalization methods, and applying the differentiability constraint to improve accuracy. Similarly, while applying the initial conservation of residuals condition had little to no effect as it does not have rational reason.

Relaxation based methods for the coupling of nonconservative hyperbolic systems
Kolbe, Niklas; Herty, Michael; Müller, Siegfried
RWTH Aachen University
17:50

We consider a relaxation system for nonconservative hyperbolic systems, in which a nonlocal source term accounts for the nonconservative product, and study its asymptotic limit. A path-conservative scheme is derived taking the discrete limit of an implicit-explicit scheme for this relaxation system. We employ both the relaxation system and the scheme to develop a new strategy for the coupling of two nonconservative systems at a static interface. In particular, we introduce new path-conservative coupling conditions and provide a corresponding Riemann solver. We show numerical experiments that apply the approach to a coupled model of blood flow through the vasculature and the two-layer shallow water system.

S18.06: Adaptive methods

Date: March 21, 2024 08:30–10:30
Room: G22/020
Chair(s): Freese, Philip

A posteriori error estimates for nonconforming discretizations of singularly perturbed biharmonic operators
Gallistl, Dietmar; Tian, Shudan
Friedrich Schiller University Jena
08:30

For the pure biharmonic equation and a biharmonic singular perturbation problem, a residual-based error estimator is introduced which applies to many existing nonconforming finite elements. The error estimator involves the local best-approximation error of the finite element function by piecewise polynomial functions of the degree determining the expected approximation order, which need not coincide with the maximal polynomial degree of the element, for example if bubble functions are used. The error estimator is shown to be reliable and locally efficient up to this polynomial best-approximation error and oscillations of the right-hand side.

A posteriori error estimates for numerical approximations of the Keller-Segel system
Giesselmann, Jan (1); Kolbe, Niklas (2); Kwon, Kiwoong (3)
1: TU Darmstadt
2: RWTH Aachen University
3: Kyungpook National University, South Korea
08:50

In this talk we review recent progress on reliable a posteriori error estimates for finite volume and discontinuous Galerkin approximations of the Keller-Segel system, one of the most famous models for chemotaxis. The error estimates are based on suitable reconstructions of numerical solutions that are combined with stability estimes. In turns out that for linear diffusion it makes sense to use stability results in the L^∞-in-time and L^2-in-space norm while for non-linear diffusion one needs to use stability results in the L^∞-in-time and H^{-1}-in-space norm. Since exact solutions may develop singularities in finite time, it is not surprising that the error estimates are conditional i.e. upper error bounds are only provided if residuals are small enough and certain norms of the numerical solution are not too large. In this constext it is interesting to note, that we can show (for linear diffusion) that if until a certain time the numerical solution is well-behaved and has small residuals then the exact solution cannot have blown-up before this time.

A-posteriori error estimates for systems of hyperbolic conservation laws

Giesselmann, Jan (1); Sikstel, Aleksey (2)
1: TU Darmstadt
2: University of Cologne

09:10

In practice, solutions of systems of hyperbolic conservation laws turn out to be of heterogeneous nature: in some regions solutions are smooth whereas in other regions discontinuities may occur. Thus, numerical simulations of these systems profit from adaptive mesh refinement avoiding waste of time and resources. To obtain a dynamic grid adaptation strategy we focus on rigorous a-posteriori error estimators.

We provide rigorous and computable a-posteriori error estimates for first order finite-volume approximations of nonlinear systems of hyperbolic conservation laws in one spatial dimension. Our estimators rely on recent stability results by Bressan, Chiri and Shen and a novel method to compute negative order norms of residuals. Numerical experiments show that the error estimator converges with the rate predicted by a-priori error estimates.

A Posteriori Error Estimation and Adaptivity for Temporal Multiscale Problems

Lautsch, Leopold; Richter, Thomas
Otto von Guericke University Magdeburg

09:30

In science and engineering, problems over multiple scales in time often arise. Two examples are material damage in oscillating structures or plaque growth in pulsating blood vessels. Here the long term effects are of interest but they depend on the coupled fast-changing physical processes which must be taken into account.

One method to efficiently simulate these problems is to split them into an averaged long term part and a localized micro scale part. We apply the dual weighted residual method on a generalized formulation for this type of problem to obtain an error estimator which can be used for adaptive refinement. Special care must be taken to separate the long term and micro scale influences on the estimator.

References

[1] S. Frei and T. Richter. Efficient approximation of flow problems with multiple scales in time. *SIAM Multiscale Modeling and Simulation*, 18(2), 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://10.1515/cmam-2021-0030)

Goal oriented error estimation for space-time adaptivity in phase-field fracture

Kosin, Viktor (1,2); Fau, Amélie (1); Hild, François (1); Wick, Thomas (2)
1: ENS Paris-Saclay, France
2: Leibniz University Hannover

09:50

In this talk, we introduce a phase-field fracture model in a space-time formulation and use the dual-weighted residual (DWR) method to formulate a goal oriented error estimator for adaptive refinement in space and time. Tensor-product space-time finite elements are being used with continuous elements in space and discontinuous elements in time, such that the primal problem can be solved with a time-stepping scheme. Because the irreversibility condition is solved using an active set method, the time dependency vanishes for the adjoint problem and no backwards time-stepping is needed. The error is localized using partition of unity (PU). The convergence order of the space-time adaptivity is analyzed on numerical tests with different goal functionals.

S18.07: Time discretisation

Date: March 21, 2024 14:00–16:00
Room: G22/020
Chair(s): Freese, Philip

Two Discretisations of the Time-Dependent Bingham Problem

Carstensen, Carsten (2); Schedensack, Mira (1)
1: Leipzig University
2: Humboldt-Universität zu Berlin

14:00

This talk introduces a non-conforming Crouzeix-Raviart approximation of the stationary three-dimensional Bingham problem and the two-dimensional Mosolov problem for the flow in a pipe. The non-conformity allows for quasi optimal error estimates in contrast to the standard conforming P1 finite element scheme. Moreover, this space discretisation is combined with two time-discretisations for the corresponding time-dependent problems. The first time discretisation is a generalised mid-point rule and the second time discretisation is a discontinuous Galerkin scheme. The a priori error analyses for both schemes yield certain convergence rates in time and optimal convergence rates in space. It guarantees convergence of the fully-discrete scheme with a discontinuous Galerkin time-discretisation for consistent initial conditions.

Time integration in spectral methods for reaction diffusion equations

Pulch, Roland
University of Greifswald

14:20

We consider initial-boundary value problems of reaction diffusion equations, which are partial differential equations in time and two space dimensions. A spectral method is used assuming periodic boundary conditions in space domain. This approach yields an initial value problem of an autonomous system of ordinary differential equations (ODEs), where the right-hand side is partitioned into a linear term and a nonlinear term. The linear term is stiff, whereas the nonlinear term is either non-stiff or mildly stiff. We investigate one-step methods for the time integration of the ODEs. On the one hand, Rosenbrock-Wanner W-methods can be applied. Therein, the Jacobian matrix of the right-hand side is replaced by an approximation, where only the linear part is included. On the other hand, a transformation using an integrating factor generates a non-autonomous system of ODEs. Now the application of explicit one-step methods like Runge-Kutta schemes is examined. We present results of numerical computations in the case of a Turing system.

Time discretisation of parabolic problems on evolving domains by means of a Crank-Nicolson scheme and implicit extensions

Frei, Stefan (1); Singh, Maneesh K (2)
1: University of Konstanz
2: Imperial College London

14:40

We consider a time-stepping scheme of Crank-Nicolson type for the heat equation on evolving domains formulated in Eulerian coordinates. As the spatial domain varies between subsequent time steps, an extension of the ”old” solution from the previous time step is required. Following Lehrenfeld & Olskanskii [ESAIM: M2AN, 53(2): 585-614, 2019], we apply a cut finite element method for spatial discretisation in combination with implicit extensions based on so-called ghost-penalty terms. In comparison to previous works for BDF time-stepping schemes, the analysis is complicated by the appearance of gradients of the ”old” extended solution on the new domain. We give some insights into priori error analysis in space and time, which results in particular in second-order convergence in time under the CFL condition $dt <= ch^{3/2}$. Finally, we present numerical results in two and three space dimensions that confirm the analytical estimates.

A Second-Order Iterative Time Integration Scheme for Linear Poroelasticity

Deiml, Matthias (1); Altmann, Robert (2)
1: University of Augsburg
2: Otto von Guericke University Magdeburg

15:00

The equations of poroelasticity appear in various application fields such as in geomechanics or medicine. They are composed of an equation for the elastic deformation of the solid and a second equation for the flow of the liquid and, hence, form a coupled elliptic–parabolic problem.

We focus on the time discretization of the spatially discretized poroelasticity model. For this, the application of fully implicit methods exhibits inefficiency due to the high dimensionality of the coupled problem. As such we consider two semi-explicit approaches, meaning that the mechanics and flow equations are solved sequentially rather than at once. On one hand, iterative methods such as the fixed-stress scheme try to approximate the fully implicit solution through an iterative matrix splitting. These approaches, however, usually lack a rigorous analysis for a fixed number of inner iterations. On the other hand, the recently introduced semi-explicit Euler method only needs to solve the mechanics and flow equations exactly once, but it is only stable if the coupling between the two equations is sufficiently weak. The semi-explicit Euler method also gives rise to a second-order scheme with even stronger coupling assumptions.

Within this talk we introduce a new family of methods combining the iterative idea with the semi-explicit Euler approach. More precisely, we consider iterative schemes with an a priori specified number of inner iteration steps depending on the coupling strength. The construction of the schemes, however, is based on the semi-explicit Euler scheme extended with an inner fixpoint iteration and an additional relaxation step. This approach gave rise to two new schemes, one with first-order and one with second-order convergence. While the convergence for an unlimited number of inner iteration steps can be shown easily, we also present an explicit upper bound for the number of iterations needed to guarantee convergence. Finally, we compare all three approaches using an example taken from medical literature.

A second order accurate in time positivity preserving scheme for a Chemotaxis system

Pervolianakis, Christos 15:20
Friedrich Schiller University Jena

We consider a Keller-Segel system which is a non-linear coupled parabolic-parabolic system for functions (u,c) on convex bounded domain $\Omega$of R^2 endowed with zero neumann boundary conditions. The Keller-Segel system describes the aggregation of slime molds resulting from their chemotactic features. The function u is the cell density of cellular slime molds while c is the concentration of the chemical substance secreted by molds themselves. It is well known that for the system, we have conservation of total mass for the function u, and the positivity preserving if the initial functions are chosen positive.

In this work, we develop numerical methods that are second-order accurate in time and at the same time the solution remains positive using a local extremum diminishing flux limiter that is also used in [3, 1].

The spatial variable is discretized by linear finite element method in quasi-uniform triangulations where all interior angles of triangles are lower or equal than $\pi/2$.

We discretize the resulting ODE system from semi-discretization with a second order explicit modified Patankar Runge-Kutta method, cf., e.g., [2] and the reference therein. We prove the uniqueness and the existence of the resulting fully discrete scheme as well as its positivity and mass conservation under the condition for the temporal and spatial mesh step, i.e., $k = O(h^{1+\varepsilon})$, $\varepsilon>0$. We also present numerical experiments, illustrating the second order accuracy in temporal variable.

[1] Chatzipantelidis, P., Pervolianakis, C. *Error analysis of a backward euler positive preserving stabilized scheme for a chemotaxis system*. arXiv:2210.04709 (2022).

[2] Kopecz, S., Meister, A. *On order conditions for modified patankar–runge–kutta schemes*. Appl. Numer. Math. 123 (2018).

[3] Strehl, R., Sokolov, A., Kuzmin, D., Turek, S.*A flux-corrected finite element method for chemotaxis problems*. Comput. Methods Appl. Math 10 (2010).

S18.08: Multiscale methods

Date: March 21, 2024 17:40–18:40
Room: G22/020
Chair(s): Freese, Philip

On a multiscale formulation for rough boundaries

Schmidt, Kersten; Pfaff, Sven 17:40
TU Darmstadt

Rough boundaries with small geometric structures often lead to high gradients and a loss of regularity concentrated in a boundary layer. The solution of elliptic equations is at some distance of the boundary only affected in an effective way. For the Poisson equation we will introduce a multiscale formulation with a macroscopic and a mesoscopic unknown in scaled coordinates. Following the method of matched asymptotic expansions in the formulation the traces of the macroscopic variable on the boundary are coupled with the behaviour of the mesoscopic unknown and its gradient in an infinite strip. We introduce a variational formulation using a Beppo-Levi space in the strip and show its well-posedness. As a further step towards a numerical method we truncate the infinite strip and estimate the truncation error. A finite element discretization of the formulation is sketched.

An adaptive stochastic Galerkin method based on multilevel expansions

Bachmayr, Markus (2); Eigel, Martin (3); Eisenmann, Henrik (2); Voulis, Igor (1) 18:00
1: University of Göttingen
2: RWTH Aachen University
3: Weierstrass Institute for Applied Analysis and Stochastics

The subject of this work is a stochastic Galerkin method for second-order elliptic partial differential equations with random diffusion coefficients. It combines operator compression in the stochastic variables with adaptive galerkin approximation in the spatial variables.

The focus of this talk is on adaptive finite element algorithms for computing sparse Legendre approximations with respect to stochastic variable of the solutions, where each Legendre coefficient is an unknown spatial function. For a suitable multilevel structure, one obtains improved convergence results for such Legendre expansions.
In an first work it was shown that by combining an adaptive operator application for the parametric expansion with independent adaptive wavelet schemes for the spatial discretizations, one can achieve optimal convergence rates at an optimal computational cost, under natural assumptions. Similar results can be developed for adaptive finite element schemes.

In this talk, we revisit these recent results and discuss ongoing developments on how to achieve similar results for schemes with adaptive spatial finite element methods discretizations. We provide a convergence analysis for the adaptive finite element method. We discuss numerical experiments which illustrate optimal or close to optimal complexity.

S18.09: Finite elements

Date: March 22, 2024 08:30–10:30
Room: G22/020
Chair(s): Wieners, Christian

Trefftz-DG for Stokes problems

Lehrenfeld, Christoph (1); Lederer, Philip Lukas (2); Stocker, Paul (3) 08:30
1: University of Göttingen
2: University of Twente, The Netherlands
3: University of Vienna, Austria

Trefftz Discontunuous Galerkin (DG) methods provide a way to reduce the computational costs of DG methods. Recently, with the introduction of weak and quasi-Trefftz DG methods, the range of applications for the Trefftz idea has increased. In this talk we consider the Trefftz idea for solving the Stokes equations. Discrete solutions of a corresponding method fulfill the Stokes equation pointwise within each element and yield element-wise divergence-free solutions. We discuss the conception, analysis and implementation of the method and present numerical examples including a compariolson with other methods.

Geometrically higher order unfitted space-time methods for PDEs on moving domains

Heimann, Fabian (1); Lehrenfeld, Christoph (1); Preuß, Janosch (2) 08:50
1: University of Göttingen
2: University College London

The methodology of unfitted finite element methods, i.e. methods that are able to cope with interfaces or boundaries that are not aligned with the grid, have been investigated for different problems in recent years, in particular for spatial problems. The benefit of flexible handling of geometries becomes especially interesting with time-depending problems on moving domains. Hence, we investigate generalisations of well-established techniques from the spatial case to the moving domain case. [1] For instance, the isoparametric mesh curvature of [2] is generalised to a space-time setting, yielding a higher order accurate discrete geometry in space and time. This gives a solution to the issue of numerical integration on implicit domains, which is one of the key challenges for unfitted methods. Another one is the stability under ill-posed cut configurations. To this end, we present a space-time version of a Ghost penalty stabilisation, which we call the direct Ghost penalty. To apply these problem-independent techniques to an example discretisation, we focus on a convection-diffusion problem and design a discontinuous in time, conforming in space Galerkin discretisation. The higher order convergence property of this method is investigated numerically and we briefly mention results from numerical analysis. [3] For computational benefits, we also introduce a continuous in time Galerkin variant. Apart from the bulk convection-diffusion problem, we also investigate a coupled convection-diffusion problem on bulk and surface.

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Analysis of a nonconformig finite element method for vector-valued Laplacians on the surface

Mehlmann, Carolin 09:10
Otto von Guericke University Magdeburg

We analyse a recently developed nonconforming surface finite element which is used to discretize 2D vector-valued compressible geophysical flow problems in a 3D domain. The study is performed on a vector-valued Laplace problem, which results from modeling surface flows. In our approach, the flow is approximated via edge integration on local flat triangles using the nonconforming linear Crouzeix-Raviart element. The approach is numerically efficient and straightforward to implement. For this discretization we derive optimal error bounds and present an estimate for the geometrical error. Numerical experiments validate the theoretical results.

On H(Curl) shape functions

Haubold, Tim (1); Beuchler, Sven (2); Schöberl, Joachim (3) 09:30
1: University of Göttingen
2: Leibniz University Hannover
3: TU Wien

In this talk, we report on some new results regarding high order H(Curl) shape functions based on Jacobi polynomials. Firstly, we show that our high order constructions on triangles and tetrahedrons are in the second Nédélec space. Secondly, we derive fast interpolation operators, which are high order functions that are L^2 dual to our shape functions. For example, those functions can be applied

to interpolate starting values of time dependent problems efficiently onto our mesh. We also give some results for high order H(Div) shape functions.

Derivation and simulation of thermoelastic Kirchhoff plates

Alms, Johanna 09:50
Leibniz University Hannover

Within the research of the Cluster of Excellence PhoenixD it is of interest to simulate thermoelastic materials on thin optical components which have the structure of Kirchhoff-Plates. This leads to a bothsided nonlinear coupled 2nd order variational system of the heat equation and the elasticity equations. The standard finite element method (FEM) is a powerful tool for the numerical solution of boundary value problems of elliptic PDEs. Because of the 2nd order of the system standard FEM cannot be applied directly. However for the biharmonic equation a mixed formulation was developed such that it is reduced to a first order variational problem. In this talk we will present a regularity result for the thermoelastic system and we derive a 1st order thermoelastic system on Kirchhoff-Plates by extending the mixed method for the biharmonic equation. This enables the Usage of standard FEM. We finish the talk with some FEM simulation results of our implementation in deal.ii.

ON THE DYNAMICS OF BLOWUP-POINTS: AN INVERSE MATRIX MODELING APPROACH FOR ESTIMATIONS ON THE NONLINEAR BEHAVIOR OF THE INCOMPRESSIBLE 3D NAVIER-STOKES EQUATION

Shadmani, Davood 10:10
University of Duisburg-Essen

This work is motivated by the need for efficient and accurate methods to understand and predict the behavior of convection-dominated scenarios for turbulent flow fields governed by the incompressible 3D Navier-Stokes system of equations, where nonlinear hyperbolic transport mechanism starts to prevail. It aims to generalize the dynamics of a blowup point in developing a matrix model as a system of equations to analyze the blowup-point formation pattern, properties, and mechanism in an inverse process, which has led to significant advances in our understanding of convection-dominated scenarios and its relation to the high regularity blowup-point for estimations on the nonlinear behavior of the incompressible 3D Navier-Stokes equation along with a correspondingly effective numerical method for its pattern-forming behavior.

The treatment method relies on some technical ideas and definitions based on the behavior of vibration modes (associated with charged particles at a blowup state) to construct a positive-definite transformation operator for the basis and structure of a successful model for a multiscale-structure description of a blowup state (in terms of properties and formation mechanism) in the sense that is consistent with the Navier-Stokes equation. Then, applying the obtained operator in the Navier-Stokes equation facilitates estimating the nonlinear term and the velocity vector field. It also reveals a behavioral interconnection between the two realms of small- and large-scale structures of an incompressible fluid for the existence and uniqueness of a solution as it continuously shifts its energy to increasingly higher frequencies or equivalently to an increasingly smaller-scale structure realm.

In conclusion, the study of blowup states is a relatively new field for which there is still much to learn about their dynamics. The inverse approach used in this study for a multiscale-structure description of a blowup-state to achieve a matrix model for the formation mechanism has yielded some promising results. Moreover, the obtained matrix model leads to a new globally bounded and scale-invariant quantity that establishes appropriate estimates on the nonlinear term for the incompressible 3D Navier-Stokes equation, either with or without a forcing term, which is a significant achievement, as the nonlinear term is notoriously difficult to estimate. Finally, this study opens up to the uniqueness of a class of globally smooth solutions with stable structures and high regularity.

The potential applications for this research are vast and can lead to significant advancements in related interdisciplinary fields of research and study.

S19: Optimization of differential equations

Organizer(s): Meinlschmidt, Hannes *(FAU Erlangen-Nürnberg)*
Rauls-Ehlert, Anne-Therese *(TU Darmstadt)*

S19.01: Various topics in Optimization of Differential Equations (1)

Date: March 19, 2024 08:30–10:30
Room: G22/211
Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

An ADMM-based time domain decomposition approach for PDE constrained optimization

Ulbrich, Stefan 08:30
TU Darmstadt

We consider optimization problems governed by time-dependent parabolic PDEs and discuss the construction of parallel solvers based on time-domain decomposition. We propose an ADMM-based approach to decompose the problem in independent subproblems and combine it with a multigrid strategy. We analyze the convergence properties and present numerical results.

On vanishing state constraints for parabolic PDEs with applications to hybrid optimal control

Kuchler, Christian; Hante, Falk 08:50
Humboldt-Universität zu Berlin

Vanishing constraints are notoriously known to provide a major challenge for many mathematical applications since they frequently violate standard constraint qualifications. Although over the years valuable insight has been gained for the associated non linear problems in finite dimensions, still little knowledge is available in the direction of infinite dimensional systems. Therefore vanishing state constraints still pose a serious task in the optimal control framework. We discuss theoretical and algorithmic approaches to optimal control problems featuring vanishing state constraints on the example of hybrid dynamical systems involving a state induced switching mechanism, since these problems can be reformulated as problems displaying vanishing state constraints. Furthermore we demonstrate the connection of vanishing constraints to the class of equilibrium constraints. Ultimately we proceed along the path of indirect methods to characterize suitable candidates for optimality and report on numerical results for a selected benchmark test.

Global minimization of polynomial integral functionals with semilinear elliptic PDE constraints

Fantuzzi, Giovanni (1); Fuentes, Federico (2) 09:10
1: FAU Erlangen-Nürnberg
2: Pontificia Universidad Católica de Chile

This talk presents a method to computationally approximate *global minimizers* for nonconvex integral functionals with polynomial integrands. The minimization is over functions in a Sobolev space that may be required to satisfy a semilinear elliptic PDE. Such problems, with or without the PDE constraints, arise in many branches of physics and engineering, such as microstructure and pattern formation. Instead of performing descent steps or producing solutions to first-order optimality conditions, the approach we present combines a discretization step with convex relaxation. Precisely, the finite element method is employed to discretize the original nonconvex variational problem into a nonconvex polynomial optimization problem (POP) with *sparse* couplings between the variables. The POP is then relaxed into a hierarchy of convex and tractable semidefinite programs (SDPs) using techniques for polynomial optimization. Optimal solutions of the SDPs provide approximations to a global minimizer of the original variational problem, and can be shown to converge to the latter under suitable assumptions. As a result, one obtains a provably convergent numerical approach to compute global minimizers for nonconvex optimization problems. The practical performance of this approach

will be showcased on examples and open questions regarding its theoretical understanding will be outlined.

Optimal control for a class of hypocoercive Fokker-Planck equations
Breiten, Tobias (1); Kunisch, Karl (2)
1: TU Berlin
2: University of Graz, RICAM Linz, Austria
09:30

The transient and long time behavior of Langevin equations has received increased attention over the last years. Difficulties arise from a lack of coercivity, usually termed hypocoercivity, of the underlying kinetic Fokker-Planck operator which is a consequence of the partially deterministic nature of a second order stochastic differential equation. Similar challenges arise within the study of the continuous version of (stochastic) Cucker-Smale type flocking models where the resulting hypocoercive PDE additionally becomes nonlinear. Introducing controls on the finite-dimensional level naturally leads to abstract infinite-dimensional bilinear control problems with an unbounded but admissible control operator. By means of an artificial diffusion approach, solutions to a class of hypoercives PDEs as well as to associated optimal control problems are analyzed under smallness assumptions on the initial data.

Adjoint-based calibration of nonlinear stochastic differential equations
Bartsch, Jan; Denk, Robert; Volkwein, Stefan
University of Konstanz
09:50

To study the nonlinear properties of complex natural phenomena, the evolution of the quantity of interest can be often represented by systems of coupled nonlinear stochastic differential equations (SDEs). These SDEs typically contain several parameters which have to be chosen carefully to match the experimental data and to validate the effectiveness of the model. In the present talk the calibration of these parameters is described by nonlinear SDE-constrained optimization problems. In the optimize-before-discretize setting a rigorous analysis is carried out to ensure the existence of optimal solutions and to derive necessary first-order optimality conditions. For the numerical solution a Monte-Carlo method is applied using parallelization strategies to compensate for the high computational time. In the numerical examples an Ornstein-Uhlenbeck and a stochastic Prandtl-Tomlinson bath model are considered.

Risk-averse optimal control of random elliptic variational inequalities
Alphonse, Amal
Weierstrass Institute for Applied Analysis and Stochastics
10:10

In this talk, I will discuss a risk-averse optimal control problem governed by an elliptic variational inequality (VI) subject to random inputs. I will derive two forms of first-order stationarity conditions for the problem by passing to the limit in a penalised and smoothed approximating control problem. The lack of regularity with respect to the uncertain parameters and complexities induced by the presence of the risk measure give rise to delicate analytical challenges seemingly unique to the stochastic setting.

S19.02: Various topics in Optimization of Differential Equations (2)

Date: March 19, 2024 16:30–18:30
Room: G22/211
Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

Control in the coefficients of an elliptic differential operator: topological derivatives and Pontryagin maximum principle

Wachsmuth, Daniel 16:30
JMU Würzburg

We investigate optimization problems, where the coefficient in the main part of the elliptic operator is the control variable. We derive the topological derivative with respect to changes in the coefficient. While the expression for the derivative is well-known, one crucial step in the proof is new. It allows for very mild assumptions on the coefficients and the domain: the derivation of the derivative works under the same assumptions than the Lax-Milgram theorem. In particular, no continuity of the coefficient or the state is assumed. This topological derivative is then used to derive a Pontryagin maximum principle. Here, an additial term arises from the topological derivative, which does not appear in the Frechet derivative.

Asymptotics and Optimal Control for Radiative Processes

Pinnau, René 16:50
RPTU Kaiserslautern-Landau

We present an asymptotic analysis for an optimal control problem constrained by the by the SP1 system for radiative heat transfer. In particular, we are interested in the asymptotic limit for optically thick materials, in which the SP1 system reduces to the well-known Rosseland approximation. The careful derivation of apriori estimates allows to show that the sequence of minimzers is indeed converging. Finally, the analytical results are underlined by numerical simulations.

Optimal Control of the Generalized Riemann Problem for Hyperbolic Systems of Conservation Laws

Breitkopf, Jannik; Ulbrich, Stefan 17:10
TU Darmstadt

In this talk, we analyze optimal control problems for quasilinear strictly hyperbolic systems of conservation laws where the control is the initial state of the system. The problem is interesting, for example, in the context of fluid mechanics or traffic flow modelling. Similar problems for scalar conservation laws have already been studied. However, the case of hyperbolic systems is more involved due to the coupling of the characteristic fields.

We begin our analysis by considering the Generalized Riemann Problem (GRP), which has a piecewise smooth initial state with exactly one discontinuity. This is a natural choice since it is well known that solutions to hyperbolic conservation laws generally develop discontinuities even for smooth data. For piecewise C^1 initial data we obtain the existence, uniqueness and stability of an entropy solution by a careful fixed point argument built on the associated Riemann Problem with piecewise constant initial states. The construction yields insights into the structure and regularity of the solution and provides a foundation to derive differentiability results of the control-to-state mapping.

The entropy solution is piecewise C^1. Its smooth parts are separated by C^2 curves which are either shock curves or boundaries of rarefaction waves. In a subsequent step, we show that these curves depend differentiably on the initial state. This allows the transformation to a reference space on a fixed space-time domain. In the reference space, we can show that the transformed solution depends differentiably on the initial state in the topology of continuous functions. This property can be translated back to the physical coordinates in the sense that the solution operator of the hyperbolic system into regions with a positive distance to shock curves or boundaries of rarefaction waves is continuously differentiable in the topology of continuous functions w.r.t. the initial state. For this, a detailed knowledge of the structure of the solution and the behaviour of the shock curves is crucial. As an immediate consequence, the differentiability of tracking type functionals for the optimal control problem follows.

A Variational Calculus for Optimal Control of Networks of Scalar Conservation or Balance Laws

Steinhardt, Marcel; Ulbrich, Stefan 17:30
TU Darmstadt

Networks of scalar conservation or balance laws are for example used in models for vehicular traffic flow, supply chains or transmission of data. These networks consist of initial boundary value problems (IBVPs) of scalar conservation or balance laws on every edge coupled in nodes by so-called node conditions. For the optimal control of solutions, a variational calculus is desirable that implies differentiability with respect to controls for objective functionals containing the solution operator. In the last decade research on IBVPs successfully introduced a variational calculus based on the concept of shift-differentiability which implies continuous Fréchet-differentiability of objective functionals of tracking type and allows to formulate an adjoint based gradient representation.

This talk presents recent progress in the extension of these results to networks of scalar conservation or balance laws. Regarding node conditions we introduce a framework for their representation which is compatible with the known approach for IBVPs on single edges and allows us to extend results on the network such as continuous Fréchet differentiability and an adjoint based gradient representation for particular functionals with respect to controls.

Semi-smooth Newton Method for parabolic PDE-constraint Optimization

Reinhold, Alexander; Urban, Karsten 17:50
Ulm University

The solution of optimization problems constrained by parabolic PDEs is highly relevant for a wide range of applications and an interesting ongoing research subject. The usual approach to numerically solve these problems is to apply time stepping schemes to the PDE and the arising adjoint equation. In our approach we utilize a space-time variational formulation, using Lebesgue-Bochner spaces. We formulate the PDE-constraint optimization problem within this framework and use a tensor type discretizations with finite elements in time and space.
Since we consider additional constraints to the control term, we will use a semi-smooth Newton method to solve the problem. In this talk we want to discuss the derivation of the arising Newton systems in our setting. Here we want to discuss the differences between a discretize-before-optimize (DBO) and the optimize-before-discretize (OBD) approach. A comparison of the Newton like method in our Petrov-Galerkin setting with the Galerkin setting of an elliptic problem is discussed as well.
Also an implementation of both approaches will be presented. For both approaches we use a tensor structure discretization. We present the numerical results showing the efficient solution of the Newton system utilizing these tensor structures.
Finally an outlook for a parameterized problem is given and we discuss the possibilities for Model Order Reduction (MOR) techniques for this problem.

Local extrema in two-phase optimal design problems

Vrdoljak, Marko; Kunštek, Petar 18:10
University of Zagreb, Croatia

We investigate optimal design problems for conductivity in two isotropic phases, each with prescribed quantities, with the goal of optimizing the energy functional. It is well-established that this problem exhibits a maximizer in the case of spherical symmetry, where the domain is either a ball or an annulus, and the right-hand side is a radial function. Specifically, the application of saddle point theory yields a unique solution, which is radial, except in specific singular cases. However, to attain this result, the initial step involves introducing a proper relaxation of the optimal design problem through homogenization theory. This process entails the introduction of generalized materials, which are mixtures of the original phases at the micro-scale.

Even in the simplest, spherically symmetric case, where the maximizer is unique, questions arise concerning its stability. Additionally, it is intriguing to explore the existence of other local extrema. We

address these inquiries through shape calculus. After expressing the first and second-order shape derivatives, the Fourier series expansion proves to be a successful technique for assessing the sign of second-order variations in critical designs. This is particularly applicable in cases of simple radial designs, where the interface between two given isotropic phases consists of a single sphere. This approach can identify local maxima different from the global one, providing insights into their presence in numerical treatments of the problem.

Conversely, for any outer heat source, the considered simple designs cannot yield a local minimum of the energy functional. We present results in a more complex scenario where the interface comprises two concentric spheres. The analogous minimization problem exhibits different behavior in the context of relaxation via homogenization theory, as generalized materials become unavoidable to reach the minimum. By introducing additional regularizing terms to the functional, such as the perimeter of the interface, the same techniques can be applied to address stability questions.

S19.03: Sparsity and nonsmooth regularization in Optimization of Differential Equations

Date: March 20, 2024 08:30–09:30
Room: G22/211
Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

DC Reformulation of Cardinality Constrained Problems in Function Spaces

Dittrich, Bastian; Wachsmuth, Daniel 08:30
JMU Würzburg

We consider cardinality constrained problems in the space of integrable functions. It is shown that this non-convex and discontinuous constraint can be equivalently reformulated by the difference of two convex and continuous functions, namely the L^1-norm and the so called largest-K norm. The convex subdifferential of the largest-K norm is calculated and optimality conditions for the penalized problem are studied. To solve the original problem practically we furthermore provide a finite dimensional exact reformulation for cardinality constraints in the space of piecewise linear functions on arbitrary triangular finite elements. An exemplary problem is solved by applying a DC method to the penalized reformulated problem, for which we also prove an exact penalty result.

Spatially sparse optimization problems

Lentz, Anna; Wachsmuth, Daniel 08:50
JMU Würzburg

We consider time-dependent optimization problems on a domain $[0,T] \times \Omega$ in fractional Sobolev spaces H^s for $s \in (0,1)$. To obtain spatially sparse solutions, the objective function contains the sparsity promoting L^p-pseudo norm for $0 < p < 1$, which makes the problem non-convex and non-smooth. In order to avoid computing the fractional Laplacian on $[0,T] \times \Omega$, we introduce an auxiliary function $w \in H^s(\Omega)$ that is an upper bound for the function $u \in L^2([0,T] \times \Omega)$. Optimality conditions and regularity results for this problem are discussed. This is done by smoothing the L^p-pseudo norm and by penalizing the inequality constraint regarding u and w.
The problem is solved numerically with a DC-like algorithm.

TV-regularized optimal switching control of PDEs by sequential relaxation

Bock de Barillas, Paulina (1); Hante, Falk (1); Hintermüller, Michael (2)

1: Humboldt-Universität zu Berlin

2: Weierstrass Institute for Applied Analysis and Stochastics

09:10

We propose an optimization approach to tackle a mixed integer control problem consisting in a parabolic partial differential equation with binary constraints on the control and nonlinear costs including a total variation regularization. The total variation regularization yields the existence of minimizers and is crucial for the proof of an exact relaxation result for the linearized problem. The optimization method is based on a trust-region algorithm that sequentially solves the linearized binary problem. We tackle the binary constraint by using the exact relaxation result on the linearized problem, that allows us to solve the relaxed problem without a rounding gap. We can then realize the minimization with first order optimality conditions and the semi-smooth Newton method. The work is motivated by the optimization of switching controls of electric transmission lines, with the background of the transition towards unsteady sustainable energy networks.

S19.04: Control, feedback and stabilization in Optimization of Differential Equations

Date: March 20, 2024 14:00–16:00

Room: G22/211

Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

On Stabilizing Model Predictive Control for Generalized Nash Equilibrium Problems

Hante, Falk (1); Schmidt, Martin (2); Topalovic, Antonia (1)

1: Humboldt-Universität zu Berlin

2: Trier University of Applied Sciences

14:00

We present a feedback scheme for non-cooperative dynamic games and investigate its stabilizing properties. The dynamic games are modeled as Generalized Nash Equilibrium Problems (GNEP), in which the shared constraint consists of time-discrete dynamic equations (e.g., sampled from a partial or ordinary differential equation), which are jointly controlled by the players' actions. Further, the individual player's objectives are interdependent and defined over a fixed time horizon. The feedback law is synthesized by moving horizon Model Predictive Control (MPC). We investigate the asymptotic stability of the resulting closed-loop dynamics. To this end, we introduce a family of auxiliary problems based on a modification of the Nikaido-Isoda function to approximate the original GNEPs. Basing the MPC scheme on these auxiliary problems instead, we derive conditions on the players' objectives, which guarantee asymptotic stability of the closed-loop if stabilizing end constraints are enforced. This analysis is based on showing that the associated optimal value function is a Lyapunov function. The theoretical results are complemented by numerical experiments.

Stabilizability of RHC for linear nonautonomous parabolic equations under uncertainty

Azmi, Behzad (1); Herrmann, Lukas (2); Kunisch, Karl (3)

1: University of Konstanz

2: Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria

3: University of Graz and Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria

14:20

In this talk, we investigate the stabilizability of linear time-varying parabolic equations with uncertain data using Receding Horizon Control (RHC). Within the RHC framework, the solution of an infinite-horizon optimal control problem is approximated through concatenating a sequence of finite-horizon ones in a receding horizon fashion. We address equations with random diffusion coefficients, explore uniform and log-normal distributions, and employ finite-dimensional controls through indicator functions (actuators) in open spatial subsets. We assess expected stabilizability based on the actuator count and establish an upper bound on RHC failure probability with respect to the number of actuators and parameter choices.

Feedback stabilization of parabolic equations. State estimation errors and model disturbances.

Rodrigues, Sergio S. 14:40
Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria

The stabilization of parabolic-like equations is inverstigated by means of a finite number of actuators. The control input is given in feedback form, thus its computation requires the knowledge of the state of the system. In general, in real world applications, this state will not be available in its entirety and an estimate will be used instead, constructed from the output of measurements provided by a finite number of sensors.

The design of feedback control operators involves the/some knowlegdge of the free dynamics.

The focus of the falk is put on the robustness of stabilizing feedback control inputs against state estimation errors and against undertainties on the free dynamics model.

Both explicitly given feedback operators and classical Riccati based feedback operators are considered.

Stabilizing and robustness performances of the feedback inputs are illustrated through results of simulations.

Convergence result of smooth approximations of feedback laws to optimal control problems with non-differentiable value function

Vásquez-Varas, Donato Maximiliano (1); Kunisch, Karl (1,2) 15:00
1: Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria
2: University of Graz

The synthesis of feedback laws for infinite horizon optimal control problems is a challenging task. It is known that classical methods for solving this problems suffer from the curse of dimensionality. For this reason, in recent years significant efforts have been dedicated to overcome this difficulty. In this regards, there is a group of techniques, based on training feedback laws involving the value function, by minimizing the average of the objective function of the control problem over a set of initial conditions. Although numerical experiments provide evidence of success with respect to the convergence of the constructed feedback laws, there only exist proofs about the convergence of these methods in the case when the value function is at least twice continuously differentiable. In this work we introduce error bounds depending on the either the C^1 norm or the semi-concavity constant of the functions of the approximating sequence produced by this methods. These error bounds together with the existence of a Lyapunov type function allow us to prove the existence of an smooth approximation of the value function when it is C^1 or semi-concave. Further, we extend this result to the Hölder continuous case by a diagonalization argument combined with the Moreau envelope. This result permits us to prove the convergence of the aforementioned techniques even if the value function is non-differentiable as long as it is at least Hölder continuous. Additionally, we provide an example of an infinite horizon optimal control problem for which the value functions is non-differentiable but Lipschitz continuous. We point out that in this example no restrictions on either the controls or the trajectories are assumed. Moreover, we present numerical experiments to exemplify the performance of the methodology.

Feedback control of parameter-dependent linear systems

Guth, Philipp A. (1); Kunisch, Karl (1,2); Rodrigues, Sergio S. (1) 15:20
1: Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria
2: University of Graz

A Riccati-based feedback mechanism is analyzed for parameter-dependent linear control systems with quadratic cost. The feedback is constructed by means of a finite ensemble of parameters from a training set. Its suboptimality with respect to the optimal feedback for each single parameter from the training ensemble is quantified.
The theoretical findings are illustrated with a set of application-motivated examples and confirming

numerical experiments, which demonstrate the robustness of the feedback against variations in the parameters.

S19.05: Shape and topology optimization in Optimization of Differential Equations (1)

Date: March 20, 2024 16:30–18:30
Room: G22/211
Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

Shape optimization for Maxwell's equations

König, Philipp 16:30
Leibniz University Hannover

Maxwell's equations provide the mathematical description for the propagation of electromagnetic waves in a given domain. Taking the domain as a variable in this setting and applying techniques from the field of optimal control, allows to determine an optimal domain to maximize a desired effect. In the context of light propagation, this approach is used to opitmize the shape of optical devices. Furhtermore, the underlying iterative optimization process enables the use of a GMRES preconditioner to circumvent the usual high computational cost inherent in this problem.

Shape Optimization by Constrained First-Order System Least Mean Approximation

Starke, Gerhard 16:50
University of Duisburg-Essen

We consider PDE constrained shape optimization problems and reformulate them as an L^p best approximation problem to the shape tensor introduced by Laurain and Sturm in [2] under divergence constraints. More precisely, it is shown that L^p distance of the above approximation problem is equal to the dual norm of the shape derivative considered as a functional on W^{1,p^*} (where $1/p + 1/p^* = 1$). This implies that for any given shape, one can evaluate its distance from being a stationary one with respect to the shape derivative by simply solving the associated L^p-type least mean approximation problem. Moreover, the Lagrange multiplier for the divergence constraint turns out to be the shape deformation of steepest descent direction. This provides a way, as an alternative to the approach by Deckelnick, Herbert and Hinze in [1], for computing shape gradients in W^{1,p^*} for $p^* > 2$. The discretization of the least mean approximation problem is done with (lowest-order) matrix-valued Raviart-Thomas finite element spaces leading to piecewise constant approximations of the shape deformation acting as Lagrange multiplier. Admissible deformations in W^{1,p^*} to be used in a shape gradient iteration are reconstructed locally. Our computational results confirm that the L^p distance of the best approximation does indeed measure the distance of the considered shape to optimality. Also confirmed by our computational tests are the observations from [1] that choosing p^* (much) larger than 2 (which means that p must be close to 1 in our best approximation problem) decreases the chance of encountering mesh degeneracy during the shape gradient iteration.

[1] K. Deckelnick, P. J. Herbert, and M. Hinze. A novel $W^{1,\infty}$ approach to shape optimisation with Lipschitz domains. ESAIM Control Optim. Calc. Var., 28:Paper No. 2, 29, 2022.

[2] A. Laurain and K. Sturm. Distributed shape derivative via averaged adjoint method and applications.
ESAIM Math. Model. Numer. Anal., 50(4):1241–1267, 2016.

[3] G. Starke. Shape optimization by constrained first-order system mean approximation. arXiv:2309.13595.

Eigenvalue Optimization for Elastic Structures with a Phase Field approach

Garcke, Harald (1); Hüttl, Paul (1); Kahle, Christian (2); Knopf, Patrik (1)
1: University of Regensburg
2: University of Koblenz

17:10

We investigate the problem of finding optimal domains for an elastic structure.
Thus we search for optimal topologies of elastic structures, such that an objective that includes eigenvalues of the elastic operator, 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.
Using the phase field function, we model the void domain as a soft material, similiar to approaches like SIMP or RAMP in density methods.
This results in a phase field variable $\varphi \in H^1(\Omega) \cap L^\infty(\Omega)$ that
encodes the domain of interest by $\varphi(x) = 1$ and
the void domain by $\varphi(x) = -1$.
Thus, although we optimize for an optimal domain, the final formulation is in the form of optimal control with pde constraints, where the phase field function serves as control, while the eigenvalue problem for the elastic operator constitutes the pde constraints.
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)].

Eigenvalue optimization with respect to shape-variation in electromagnetic cavities

Herter, Christine (1); Schöps, Sebastian (2); Wollner, Winnifried (1)
1: Universität Hamburg
2: TU Darmstadt

17:30

In this talk, we consider a freeform optimization problem of eigenvalues in a particle accelerator cavity by means of shape-variations with respect to small deformations. As constraint we utilize the mixed variational formulation by Kikuchi of the normalized Maxwell's time-harmonic eigenvalue problem. For the eigenvalue optimization, we apply the method of mappings. We show results of continuity and differentiablility of the eigenvalues and the associated eigenfunctions. Further, we derive an optimality system and the reduced cost functional by using the adjoint calculus. In addition, to solve the considered optimization problem, we present a damped inverse BFGS method. We conclude with two numerical examples, which show the functionality of the optimization method, and with an outlook where we explain ongoing work and further ideas to extend the usability of this mathematical approach to real-life problems.

Computing Multiple Local Minimizers of Topology Optimization Problems and Application for Hydrogen Electrolysis Cell Design

Baeck, Leon Niklas (1); Blauth, Sebastian (1); Leithäuser, Christian (1); Pinnau, René (2); Sturm, Kevin (3)
1: Fraunhofer ITWM
2: RPTU Kaiserslautern-Landau
3: TU Wien

17:50

Topology Optimization considers the optimization of a domain by changing its geometric properties by either adding or removing material. Typically, topology optimization problems feature multiple local minimizers. In order to guarantee convergence to local minimizers that perform best globally, it is important to identify multiple local minimizers of topology optimization problems. Moreover, finding local solutions that are desirable from an application standpoint due to easy manufacturability or aesthetic designs also requires the discovery of multiple local minimizers.

In this talk, we present a novel deflation approach to systematically find local minimizers of topology optimization problems. The approach is based on a penalization of previously found local solutions in the objective. Through a series of examples, including the optimization of fluids in Stokes flow and

the optimization of bipolar plates in hydrogen electrolysis cells, we demonstrate the effectiveness of our approach.

Analysis of an optimization problem for a piezoelectric energy harvester
Kaltenbacher, Barbara; Krejci, Pavel
University of Klagenfurt, Austria
18:10

The problem of optimal energy harvesting for a piezoelectric element driven by mechanical vibrations is stated in terms of an ODE system with hysteresis under the time derivative coupling a mechanical oscillator with an electric circuit with or without inductance. In the piezoelectric constitutive law, both the self-similar piezoelectric butterfly character of the hysteresis curves and feedback effects are taken into account in a thermodynamically consistent way.

The physical parameters of the harvester are chosen to be the control variable, and the goal is to maximize the harvested energy for a given mechanical load and a given time interval.

If hysteresis is modeled by the Preisach operator, the system is shown to be well-posed with continuous data dependence. For the special case of the play operator, we derive first order necessary optimality conditions and an explicit form of the gradient of the total harvested energy functional in terms of solutions to the adjoint system.

Joint work with Pavel Kerjci, CAS

S19.06: Numerical analysis and parameter identification in Optimization of Differential Equations

Date: March 21, 2024 08:30–10:30
Room: G22/211
Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

Numerical Analysis for Dirichlet Optimal Control Problems on Convex Polyhedral Domains
Vexler, Boris; Pfefferer, Johannes
Technical University of Munich
08:30

We present novel numerical analysis for discretization of Dirichlet boundary control problems. The technique is based on weighted error estimates and provides optimal order estimates for problems formulated on two- and three-dimensional polyhedral domains.

Numerical analysis of optimal control problem along curves in three dimensions.
Leykekhman, Dmitriy; Vexler, Boris
University of Connecticut, USA
08:50

In the recent years the problem of finite elment approximation and analysis of elliptic problems where the forcing function is supported on a lower dimensional manifold, like a point or a curve in three dimensions Euclidian space have received a sertain attention. There are many interesting and insightful results in this direction. However, the known results are not sufficient for obtaining optimal error estimates for optimal control problem with controls acting on curves in three dimensions. To obtain optimal (or nearly optimal) error estimates, we establish new weighted error estimates for the elliptic problems and applied them to the optimal control problems. In some sense, the established results generalized the technique of pointwise finite element error etsimates.

Error Estimates for Optimal Control of the Instationary Navier-Stokes Equations Subject to State Constraints

Vexler, Boris; Wagner, Jakob 09:10
Technical University of Munich

In this talk, we will consider an optimal control problem subject to the instationary Navier-Stokes equations with state constraints pointwise in time. The equations are approximated by a discontinuous Galerkin method in time and inf-sup stable finite elements in space. The variational nature of this discretization, on the one hand, lends itself to the treatment of optimal control problems and, on the other hand, allows for duality techniques in the derivation of error estimates for the state equation in various norms. A special discrete Gronwall lemma facilitates the analysis of discrete dual problems with right hand sides that are only L1 in time. This is needed for the derivation of an error estimate in the timewise L-infinity norm, which is of particular importance for this problem, due to the structure of the state constraint. All presented error estimates are of best approximation type, i.e., exhibit, up to a logarithmic term, optimal orders of convergence with respect to the spatial discretization parameter h and the time discretization parameter k. Compared to many results in the literature, in which different spatiotemporal norms are being estimated simultaneously, our estimates bound the error in each norm individually and thus do not exhibit an order reduction. The low required regularity on the data makes these estimates especially applicable for optimal control problems, where the regularity of the control has to be determined from the optimality conditions. From the error estimates for the state equation, we deduce estimates for the optimal control problem, while also drawing comparisons to the corresponding problem subject to the Stokes equations.

Adaptive Reduced Basis Trust Region Methods for Parameter Identification Problems

Kartmann, Michael (1); Keil, Tim (2); Ohlberger, Mario (2); Volkwein, Stefan (1); Kaltenbacher, Barbara (3) 09:30
1: University of Konstanz
2: University of Münster
3: University of Klagenfurt, Austria

In this talk, we are concerned with model order reduction in the context of iterative regularization methods for the solution of inverse problems arising from parameter identification in elliptic partial differential equations. Such methods typically require a large number of forward solutions, which makes the use of the reduced basis method attractive to reduce computational complexity.
However, the considered inverse problems are typically ill-posed due to their infinite-dimensional parameter space. Moreover, the infinite-dimensional parameter space makes it impossible to build and certify classical reduced-order models efficiently in a so-called "offline phase". We thus propose a new algorithm that adaptively builds a reduced parameter space in the online phase. The enrichment of the reduced parameter space is naturally inherited from the Tikhonov regularization within an iteratively regularized Gauß-Newton method.
Finally, the adaptive parameter space reduction is combined with a certified reduced basis state space reduction within an adaptive error-aware trust region framework. Numerical experiments are presented to show the efficiency of the combined parameter and state space reduction for inverse parameter identification problems with distributed reaction or diffusion coefficients.

Identification of the basal drag parameter in ice sheet models using L-curves

Höyns, Lea-Sophie (1,2); Kleiner, Thomas (1); Rademacher, Andreas (2); Rückamp, Martin (3); Wolovick, Michael (1); Humbert, Angelika (1,2) 09:50
1: Alfred Wegener Institute Bremerhaven
2: University of Bremen
3: Bavarian Academy of Sciences and Humanities, Munich

The West Antarctic Ice Sheet (WAIS) is currently the major contributor to sea-level change from Antarctica. One challenge in making realistic projections of future ice sheet behaviour is the unknown distribution of basal friction underneath the ice sheet. The friction has a strong influence on sliding

and, thus, an impact on ice flow speeds. Its distribution is required as an initial stress state for ice sheet models. The objective that arises is to infer the basal friction parameter – here, a parameter identification problem occurs.

The Ice-sheet and Sea-level System Model (ISSM) is used to infer WAIS basal friction parameters based on surface velocity observations. Our model equations represent the ice dynamics in an approximated way. For the boundary condition at the ice-base interface, we use a (non-)linear Budd-type friction law. This law describes the basal friction as a power-law function of sliding velocity and the effective pressure of the basal water system, with the basal friction parameter, inferred by the parameter identification. To achieve more realistic results, the effective pressure is taken from a physical-based subglacial hydrology model, the Confined-Unconfined Aquifer System model (CUAS-MPI).

The problem is solved by performing an optimization based on an L-BFGS algorithm and using adjoint equations. Our algorithm minimizes a cost function that consists of an observational term quantifying the misfit between the modeled and the observed surface velocity, and a regularization term that penalizes unrealistic oscillations in the basal friction parameter. The optimal weighting between these two cost function terms is determined by an L-curve analysis. In this L-curve experiment, we test 25 different weights, and perform a parameter identification for each sample.

Here, we focus on the challenge of dealing with these L-curves regarding the application of glaciology. The resulting L-curves are often poorly shaped with many outliers. We observed that numerical instabilities or even complex structures like rock outcrops in the ice sheet are often the cause of these problems. We are also investigating this issue in the L-curves of other parts of the Antarctic Ice Sheet.

We present our approach to parameter identification, the conduction of the L-curve analysis and how we deal with ill-formed curves. Further, our latest model results, as well as the resulting L-curve and comparison to results of other regions in Antarctica are shown.

Parameter identification of ice rheology and bottom friction for glaciers
Schmidt, Niko 10:10
Kiel University

The p-Stokes equations are nonlinear partial differential equations, used, e.g., to simulate the Antarctic or Greenland ice sheets. However, difficulties occur due to unknown physical quantities, like the ice rheology and the basal friction. The problem is identifying these physical quantities by knowing the surface velocity of the glacier from observations. Here, a parameter identification problem arises. In the mathematical literature are proofs for the existence of an optimal control and the Gâteaux differentiability of the control-to-state operator for the distributed control problem. These results are obtained by adding a small diffusion term. We extend these results to the parameter identification problem.

S19.07: Shape and topology optimization in Optimization of Differential Equations (2)

Date: March 21, 2024 14:00–16:00
Room: G22/211
Chair(s): Meinlschmidt, Hannes
Rauls-Ehlert, Anne-Therese

Robust PDE Constrained Design Optimization of Electrical Machines with Isogeometric Analysis
Komann, Theodor; Ulbrich, Stefan 14:00
TU Darmstadt

In the dynamically advancing domain of electrical machine design, the optimization of geometry and associated parameters under the presence of uncertainties constitutes a significant challenge. In this talk we propose a methodology for the combined parameter and shape optimization under uncertainty with application to 3 phase 6 pole Permanent Magnet Synchronous Machine.

The geometry is reconstructed in a two-dimensional framework within Matlab by employing Isogeometric Analysis to enable free shape optimization. The main contributions of this research are twofold. First, we combine shape optimization and parameter optimization to enhance the performance of PMSM designs. Second, to ensure these designs withstand uncertainties in operational conditions and manufacturing processes, we apply a robust optimization approach, leading to a min-max problem formulation. To solve this bilevel problem efficiently, we work with the value functions of the inner problems and apply Danskin's Theorem for the computation of generalized derivatives. Additionally, the adjoint method is employed for the efficient calculation of necessary derivatives. The paper concludes by presenting numerical results that demonstrate the effectiveness of the proposed robust optimization framework. These results indicate that our optimized PMSM designs not only perform competitively compared to non-robust counterparts but also show resilience to operational and manufacturing uncertainties, making them suitable for industrial applications.

Riemannian shape optimization of thin shells using isogeometric analysis

Rosandi, Rozan; Simeon, Bernd
RPTU Kaiserslautern-Landau

14:20

Structural optimization is concerned with finding an optimal design for a structure under mechanical load. In this contribution, we consider thin elastic shell structures [1] based on a linearized shell model of Koiter's type, whose shape can be described by a surface embedded in three-dimensional space. We regard the set of unparametrized embeddings of the surface as an infinite-dimensional Riemannian shape manifold [2] and perform optimization in this setting using the Riemannian shape gradient [3]. Non-uniform rational B-splines (NURBS) are employed to discretize the middle surface and numerically solve the underlying equations that govern the mechanical behavior of the shell via isogeometric analysis [4]. By representing NURBS patches as B-spline patches in real projective space, NURBS weights can also be incorporated into the optimization routine. We discuss the practical implementation of the method and demonstrate our approach on the compliance minimization of a half-cylindrical shell under static load and fixed area constraint. For numerical experiments, we use the GeoPDEs package [5] in MATLAB, extended by the computation of shape sensitivities and Riemannian shape optimization methods.

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Shape optimization on Riemannian manifolds including nonsmoothness

Suchan, Tim (1); Schulz, Volker (2); Welker, Kathrin (3)

1: Helmut Schmidt University, University of the Federal Armed Forces Hamburg
2: Trier University of Applied Sciences
3: TU Bergakademie Freiberg

14:40

The field of shape optimization has enjoyed significant interest from both the theoretical as well as the applied point of view. Using differential-geometric topics to approach optimization on infinite-dimensional Riemannian manifolds frequently occurs if mesh independence of the result is desired and has been the topic of recent publications. If these problems contain nonsmoothness then the numerical treatment becomes especially challenging, which will be the focus of this presentation. In this talk, we present the theoretical framework for constrained optimization in Riemannian shape spaces and demonstrate numerical applications and results of exemplary optimization problems.

A Trust-Region Method for p-Harmonic Shape Optimization

Wyschka, Henrik (1); Wollner, Winnifried (1); Rung, Thomas (2)

1: Universität Hamburg
2: Hamburg University of Technology

15:00

Recent developments in shape optimization showed improved results by using descent directions in Banach spaces, in particular by a p-harmonic approach. Here, for each outer iteration a corresponding vector-valued p-Laplace problem with boundary forcing has to be solved for possibly high-order p. Therefore, we work with an algorithm based on an interior-point method that does not require an iteration over increasing p. Extending this, we aim to also reduce the number of outer iterations and thus calls of the algorithm by proposing a trust-region method. Due to the structure of the algorithm, we are able to introduce a constraint on the gradient naturally. This results in a deformation field which fulfills a trust-region-radius in terms of the seminorm. Consequently, no further scaling during the mesh deformation process is required and potential backtracking is avoided. Moreover, in contrast to methods based on sensitivity scaling, the resulting scaling of the deformation field does not depend on the order p and also holds when considering the limit setting.

Constrained Best Approximation of Symmetric Shape Tensors and its Role for the Determination of Shape Gradients

Hetzel, Laura; Starke, Gerhard

University of Duisburg-Essen

15:20

A crucial issue in numerically solving PDE-constrained shape optimization problems is avoiding mesh degeneracy. Recently, there were two suggested approaches to tackle this problem: (i) departing from the Hilbert space towards the Lipschitz topology approximated by W^{1,p^*} (where $1/p+1/p^*=1$) with $p>2$ and (ii) using the symmetric rather than the full gradient to define a norm.
In this talk we will discuss an approach that allows to combine both. It is based on our earlier work [2] on the L^p approximation of the shape tensor of Laurain & Sturm [1]. We extend this by adding a symmetry constraint to the derived L^p best approximation problem and show that the distance measured in a suitably weighted L^p-norm is equal to the dual norm of the shape derivative with respect to the L^{p^*}-norm associated with the linear elastic strain of the deformation. Moreover, it turns out that the Lagrange multiplicator associated with the divergence constraint is the direction of the steepest descent with respect to the utilized norm. This provides a way to compute shape gradients in W^{1,p^*} with respect to the norm defined by the symmetric gradient.
The discretization of the resulting least mean problem can be done by the PEERS element and its three-dimensional counterpart.

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Shape Optimization of a Bipolar Plate using a Dimension Reduction Approach

Blauth, Sebastian (1); Leithäuser, Christian (1); O'Reilly, Cymoen (1); Pinnau, René (2)

1: Fraunhofer ITWM

2: RPTU Kaiserslautern-Landau

15:40

Hydrogen technologies play a crucial role in achieving climate-neutral mobility and fostering a clean energy industry. Electrolysis cells are used to produce hydrogen by splitting water into hydrogen and oxygen, utilizing green energy sources. This process is vital for transitioning to the widespread industrial use of clean energy. The flow dynamics of bipolar plates are essential for optimizing the performance of proton exchange membrane (PEM) electrolysis cells.

Our approach focuses on developing innovative designs to enhance the performance of PEM electrolysis cells by utilizing shape optimization techniques. Specifically, we aim to optimize the flow field and transport layer on the anode side of the bipolar plate. To minimize computational effort, we employ a dimension reduction approach for the Stokes and Stokes-Brinkman equations. The ultimate goal is to achieve a uniform flow distribution throughout the bipolar plate and porous medium while considering factors such as manufacturability and physical constraints.

S20: Dynamics and control

Organizer(s): Gehring, Nicole *(Johannes Kepler University Linz)*
Philipp, Friedrich *(Technische Universität Ilmenau)*

S20.01: Optimal control

Date: March 19, 2024 08:30–10:30
Room: G22/122
Chair(s): Flaßkamp, Kathrin
Grushkovskaya, Victoria

Gradient-free control algorithms for convex optimization problems

Grushkovskaya, Victoria 08:30
University of Klagenfurt, Austria

The presentation focuses on stabilizing a control system at the solution of a convex optimization problem, wherein the goal is to minimize an objective function under several constraints. It is assumed that the cost and constrained functions are dependent on the output of the system. Employing extremum seeking techniques, we introduce a family of controllers designed to steer a system to the set of saddle points of the associated Lagrangian.The resulting algorithm comprises control loops for both the states of a system and Lagrangian multipliers. Notably, It is derivative-free, i.e. relies only on the Lagrangian values. However, the behaviour of the resulting system resembles the dynamics of a gradient-like flow of the Lagrangian. The main result of the presentation states the practical uniform asymptotic stability of the set of saddle points. Initially, we consider so-called static systems, where the output depends only on the control values. Then the proposed approach is extended to dynamic systems with state-dependent outputs. The obtained results are illustrated with several examples, and various types of controllers are discussed.

A port-Hamiltonian perspective on energy-optimal control of adaptive high-rise buildings

Oppeneiger, Benedikt Florian (1); Zeller, Amelie (2); Schaller, Manuel (1); Worthmann, Karl (1); Sawodny, Oliver (2); Tarin, Cristina (2); Böhm, Michael (2) 08:50
1: TU Ilmenau
2: University of Stuttgart

Adaptive high-rise buildings incorporate active damping of vibrations caused by external loads such as wind or earthquakes. This allows for a significant reduction of the resource consumption during the construction process. In [1], adaptive buildings were modeled in a port-Hamiltonian way. Such port-Hamiltonian models can, e.g., be used for the design of controllers and/or observers to achieve vibration
damping [2]. We present a framework in which we take the port-Hamiltonian structure into account to allow for energy-optimal operation of adaptive high-rise buildings [3]. Moreover, we show by numerical simulations that the resulting MPC closed-loop behaviour is superior in comparison to state-of-the-art LQR-based control.
References
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Optimized Self-Consumption of Renewable Energies with Forecast-Based Energy Management for Agricultural Farms

Dierkes, Eva (1); Kappertz, Lars (2); Solovievskyi, Viacheslav (1); Hackenberg, Annika (2); Büskens, Christof (2)

1: Steinbeis Innovation Center for Optimization and Control
2: Center for Industrial Mathematics, University of Bremen

09:10

As energy costs continue to rise, owners of renewable energy sources like photovoltaic (PV) or wind power plants realize that selling energy back to the grid may not be as profitable as consuming the energy themselves. Although controlling the energy generation is not feasible for weather-dependent power plants, it is possible to predict the amount of energy produced. Self-sufficiency can be improved by regulating individual devices and storage units based on anticipated energy production and demand. For electricity tariffs much larger than feed-in tariffs, such demand-side management can notably improve the profitability of private renewable energy systems.

The project SmartFarm2 focuses on agricultural farms as a use case, given their significant energy requirements and frequent use of renewable energy. A forecast-based energy management system (EMS) is to be developed to enable automated, intelligent decision-making and control over individual devices with the goal of maximizing self-consumption. On the energy consumer side, this work considers thermal storages like milk-cooling systems and heat pumps and profile-based devices such as washing machines. For energy generation, a PV plant is considered along with a battery serving as electrical energy storage (EES). All these devices are modeled based on measured data so that forecasts of their behavior can be used for intelligent control.

This contribution is focused on the formulation of the EMS as an optimal control problem. The problem formulation differentiates between shift-able and continuously controllable devices, with a particular emphasis on the different formulations and constraints necessary within a time-discretized setting. The EMS is based on long-term predictions that enable high-level control decisions, as well as specific controls for the next controlling steps on a low level. In order to evaluate both cost function and constraints for the next prediction horizon, weather forecasts and forecasts of the power demand and state behavior of each device are considered.

This contribution demonstrates how a forecast-based EMS can be formulated and implemented with numerical optimization methods. It is simulated using a rolling horizon approach to allow for analysis in a realistic setting. The approach involves continuously gathering new data and reevaluating decisions, resulting in a dynamic system that can adapt to changes in energy production and demand.

Robust and Efficient Hybrid Optimal Control via Gaussian Process Regression and Multiple Shooting with Experimental Validation on a Double Pendulum on a Cart

Hesse, Michael; Timmermann, Julia; Trächtler, Ansgar

Heinz Nixdorf Institute, Paderborn

09:30

In this contribution, we propose an innovative method for determining optimal control sequences for nonlinear systems with partially unknown dynamics, which further expands our previous work [1]. Within the paradigm of model-based design, where the practicality and safety of commissioning feed-forward controls and closed-loop controllers have priority, our approach leverages probabilistic Gaussian Processes to adjust for model inaccuracies directly from measured system data. This differs from conventional approaches that involve complicated analytical modeling and may entail a substantial time investment to acquire expertise. Consequently, we address the limitations inherent in traditional design methodologies.

Our research focuses on the formulation and solution of the hybrid optimal control problem using probabilistic state predictions and multiple shooting. This ensures adaptability, data efficiency, and resilience against uncertainties in system dynamics. These attributes are empirically substantiated through experimental validation on a chaotic and highly sensitive dynamical system - a double pendulum on a cart.

Our methodology unfolds as an iterative learning process, systematically exploring diverse controls, accumulating valuable data within each iteration, and refining the control strategy until the desired task is accomplished. The adoption of the two-degree-of-freedom control structure allows for the distinct consideration of the feed-forward control and the closed-loop controller. For the latter, we employ a time-variant LQR designed to stabilize the system around its target trajectory. Furthermore, we integrate a probabilistic long-term prediction through linearization and the Unscented Transform, enabling systematic anticipation of safety-critical violations. Detailed insights into relevant implementation aspects are provided.

To ascertain the real-world applicability, we present an exemplary application involving a double pendulum on a cart. The objective is to bring the pendulum arms from the lower stable to the upper unstable equilibrium by horizontally moving the cart and subsequently stabilize them. In this scenario, we assume that the centrifugal forces, crucial to the system dynamics, have not been accurately modeled and must be learned from data. Experimental results are comprehensively analyzed in both simulation and real-world settings. Notably, in simulation a correction of the model error is achieved after only 2 attempts, and only 3 further attempts are necessary on the real system before the successful realization of the control task. This marks a significant improvement, surpassing our previous work in [2], where we used the purely data-driven PILCO framework and required 27 attempts, showcasing an increase of over 80% in efficiency and demonstrates significant practical applicability for commissioning control systems.

Optimal trajectories for a Dubins vehicle in mode-target games

Pedrosa, Matheus V. A. (1); Schmuck, Anne-Kathrin (2); Flaßkamp, Kathrin (1)
1: Saarland University
2: Max Planck Institute for Software Systems, Kaiserslautern

09:50

In the last decades, the synthesis of feedback controllers for non-linear systems that satisfy temporal logic specifications has been actively investigated. This is of interest, in particular, for safety-critical cyber-physical systems. The literature offers a variety of approaches for computing admissible solutions, however, the problem of finding optimal solutions is an open question that we intend to shed light on in this work. In particular, we design optimal winning strategies in a two-player game (resulting from a temporal logic specification), called mode-target game, motivated by applications in path planning. Here, an ego-robot is playing against the environment, the second player, who can trigger an infinite set of different modes, each corresponding to a different target location in the robot's state space, and this at any point in (continuous) time. Our controller synthesis technique exploits intrinsic properties of the Dubins path to find explicit optimal solutions given only the initial and the desired final positions at any point in time. Our results show that in controller synthesis under temporal logical constraints, in addition to respecting temporal rules, optimal solutions can also be found at any time in (near) real-time for the considered restricted scenario.

Commutator-free based on Cayley transform for quantum optimal control problems

Wembe, Boris (1); Maslosvkaya, Sofya (1); Ober-Blöbaum, Sina (1); Offen, Chritian (1); Singh, Pranav (2)
1: University of Paderborn
2: University of Bath, UK

10:10

Controlling complex quantum dynamics is a recurring theme in many different fields of atomic, molecular, and optical physics and physical chemistry. Recent examples include quantum state preparation, imaging or reaction control, Boson Sampling. The central idea of quantum control is to employ external fields to steer the dynamics in a desired way (see for instance C.P Koch et al. 2022). The development of fast, robust and accurate methods for the optimal control of quantum systems comprising interacting particles is one of the most active topics. Although there is a significant set of algorithms for numerical applications in the field of quantum control, the high computational cost remains a challenge for many of them. Indeed, one of the main issues is often how to efficiently integrate controlled dynamics (control necessarily implies a time-dependent Hamiltonian). Methods based on Magnus expansion coupled with splitting methods yield pretty good results in this context,

although these involve the computation of commutators (from the Magnus expansion) and several matrix exponential, which are generally costly. Our aim is then to use the Cayley transform coupled with the Magnus expansion and the commutator-free approach introduced in Alvermann & Fehske 2011 to provide high-order methods that avoid both commutator and matrix exponential computations. The use of Cayley transform being possible thanks to the nice quadratic property of quantum operators.

S20.02: Modelling & identification

Date: March 19, 2024 16:30–18:30
Room: G22/122
Chair(s): Eberle, Robert
KUCZMA, Mieczyslaw Sylwester

Modelling Gas Networks with Compressor Stations: A Port-Hamiltonian Approach

Bendokat, Thomas; Benner, Peter; Grundel, Sara; Nayak, Ashwin Sadanand 16:30
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Transportation of hydrogen across new and repurposed pipeline infrastructure is a vital pin in Germany's energy policy. Efficient network operation requires an in-depth study into the flow of gas within the network and its components. A pipeline network comprises of large pipelines connected at junctions with compressor stations compensating for the drop in fluid pressure. Transient simulation of gas networks can aid greatly in design and monitoring of a network, and the topic is studied extensively in literature [2, 3]. Network simulation models have generally emphasized on connected pipeline flow models with only recent studies focusing on including compressor models [1, 5, 7]. Compression costs for hydrogen, natural gas and their blends can differ vastly [8] and an integrated model of networks with compressors is essential for network design and control. Typical models of compressor stations are based on their power ratings, whereas some models consider it as a node with the pressure scaled by a compression ratio [1, 4] or as a pipe with negative friction [6]. In this study we follow an energy-based modelling viewpoint considering that gas networks fit into a port-Hamiltonian framework [3, 6], for which geometric integration methods can be used, preserving the structure. We evaluate gas network models with compressors specifically in this context and provide illustrative numerical examples.

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Behaviour of frame structures with pseudoelastic shape memory alloy damping elements

Kuczma, Mieczyslaw; Łasecka-Plura, Magdalena; Tabrizikahou, Alireza; Białasik, Jan 16:50
Poznan University of Technology, Poland

This contribution is concerned with the development and modelling of frame structures exposed to earthquake loading or other dynamic loading. Presented will be a model of frame structural systems which are capable of damping out vibrations. The system consists of two types of structural members or energy transformation device that work together to fulfil the requirement on the load-carrying capacity and that on the deformation. The role of dissipating and absorbing the energy induced in the system by ground motions is played by some structural members or devices made of pseudoelastic shape memory alloys which exhibit characteristic flag-shaped hysteresis loops. This structural design with a damping mechanism provides passive motion control. The motion of such a continuous structural system is governed by partial differential equations supplemented by inequality constraints which express the martensitic phase transformation criteria. The constraints are imposed on the phase transformation driving force and its thermodynamically conjugate variable (volume fraction of martensite) that describe the reversible transformation process austenite-martensite-austenite, which finally leads to the hysteresis loops.

The finite element method is used for the space discretization of the continuous structural system. The hysteretic behaviour in time of the structural system is determined incrementally by solving a sequence of complementarity problems. The obtained results of numerical simulations will be presented which demonstrate the behaviour and damping effectiveness of the proposed structural design.

Frequency response function for systems incorporating viscoelastic elements with uncertain-but-bounded parameters

Łasecka-Plura, Magdalena; Kuczma, Mieczyslaw 17:10
Poznan University of Technology, Poland

One of the important tools in the dynamic analysis of structures is the frequency response function, which allows determining the system's response to signals of different frequencies. This paper presents a method for determining the frequency response function for systems that include viscoelastic elements with design parameters specified as uncertain but within certain limits. Introducing uncertainties in parameters in the analysis and design of structures is crucial for effectively predicting system behavior under various operating scenarios.

Uncertainties in design parameters can be described using a probabilistic or interval approach. In the probabilistic approach, probability distributions are used to model uncertainties. However, for parameters describing viscoelastic material, it is often easier to define the range of their variability. In such cases, interval analysis is applied.

In this work, design parameters are described using interval numbers. To determine the frequency response function, in the first step, the equations of motion are written for systems with damping viscoelastic elements. The behavior of viscoelastic elements is described using classical and fractional rheological models. In the next step of the analysis, after applying the Fourier transform, a system of linear interval equations is obtained, and its solution comprises elements of a matrix containing the frequency response function. The fixed point iteration method is employed to solve the system of interval equations. One of the disadvantages of using direct interval arithmetic is the overestimation of results. This follows from the overlapping influences of uncertainties in individual parameters and the fact that each element of the equation is treated as an independent interval number, even if it associated with the same physical quantity. In many cases, this leads to entirely incorrect results. To eliminate these drawbacks, the element-by-element equation representation method is applied.

The obtained results will be compared with the vertex method, which, although very time-consuming, allows finding solutions for all combinations of bottom and upper bounds of design parameters. It is assumed that this method provides results close to exact solutions and can be used as a comparative one.

The proposed method of considering uncertain design parameters in systems with viscoelastic elements yields very good results in the form of limit values of the frequency response function. It is relatively simple to implement and more efficient than other methods based, for example, on derivatives calculated with respect to the changing parameter.

Estimation of nonparametric restoring forces for nonlinear mechanical single-degree-of-freedom systems: a robust and effective approach

Eberle, Robert
University of Innsbruck

17:30

Single-degree-of-freedom (SDOF) systems are a simple but widely used method in engineering to describe mechanical phenomena. Mathematically, a SDOF system can be described by a second-order differential equation (Newton's second law). In general, the differential equation depends on arbitrary parameters (e.g. spring stiffness, damping, friction), which have to be estimated from measurements.

Parameter estimation of such models is still a broad research field, especially for nonlinear systems. A widely used method for parameter estimation is the restoring force method.

A robust and computationally effective method for the determination of unknown nonparametric restoring forces for nonlinear SDOF systems based on measured data will be presented in this work. The parameter estimation problem is formulated as an inverse problem, which is solved efficiently based on the calculus of variations. The inverse problem is transformed into an efficiently solvable boundary value problem, instead of solving a complex and computationally intensive optimization problem.

The method has been successfully demonstrated in several numerical examples of nonlinear SDOF.

S20.03: System analysis

Date: March 20, 2024 08:30–09:30
Room: G22/122
Chair(s): Zuyev, Alexander
Röbenack, Klaus

A Note on the Local Observability of Uniform Hypergraphs

Gerbet, Daniel; Röbenack, Klaus
TU Dresden

08:30

Hypergraphs generalize graphs in such a way that edges may connect any number of nodes. If all edges are adjacent to the same number of nodes, the hypergraph is called uniform. Thus, a graph is a 2-uniform hypergraph. Each uniform hypergraph can be identified with an autonomous dynamical state-space system, whose vector field is composed of homogeneous polynomials. We consider the observability of dynamical systems, which possess this special structure.

In control theory, the observability of a dynamical system asks for the possibility to reconstruct the systems state from an output trajectory, where the output is a projective measurement of the systems state. In addition, one can ask for the observable subspace of the state. Nonlinear systems, although observable at almost all points in the state space, may possess not locally observable ones. The existence and location of such states are important for observability analysis and observer design.

Recently, the observability of these hypergraph systems have been studied for the general case. We apply an extended deterministic observability test to uniform hypergraphs and compute also the not observable states for different linear output maps. We are able to confirm the results of the recent study, at least for graphs with a small number of nodes due to computational complexity of our method. In addition, the not locally observable states are computed for different combinations of measured nodes.

On the Observation of Glucose-Insulin Models

Röbenack, Klaus; Gerbet, Daniel
TU Dresden

08:50

The glucose-insulin subsystem has been modelled in different ways as a low-dimensional dynamical system. These models consist of various parameters, which are fitted such that the model coincides with specific experiments. For individuals with the Diabetes Mellitus syndrome model-based controllers for insulin injection have been proposed. These controllers, however, require the knowledge of the model parameters as well as the full systems state, which must be estimated as well. In addition, the system is disturbed by in general unknown carbohydrate intake.
From a control-theoretic point of view, the state estimation using only the measurable glucose concentration is an observer problem. Due to the nonlinearity of the system, its observability is more difficult to test. There may also be some points in the state space, where the system is not locally observable for some parameters tuples. Those issues are important for a robust observer design.
We test the nonlinear observability of some selected so called short term glucose-insulin models with different complexity and discuss their observability properties. To this end, only finite-dimensional models with smooth vector field can be handled by our algebraic methods. Finally, observers for these systems are discussed.

Artifacts arising in Harmonic Balance solutions of the softening Duffing oscillator

Dänschel, Hannes (1); Lentz, Lukas (2)
1: TU Berlin
2: Trier University of Applied Sciences

09:10

For the softening Duffing oscillator with a cubic nonlinearity and harmonic excitation we perform a bifurcation analysis to obtain the system's frequency response over a given range of excitation frequencies. The approximate solution of the system obtained from the Harmonic Balance Method (HBM) yields a nonlinear algebraic equation system. An algorithmic implementation is presented that generates the resulting system which is then solved via numerical continuation as implemented in an embedded global quasi-Gauss-Newton method. The convergence behavior of the system's frequency response with respect to the HBM ansatz order is studied as well as solution artifacts arising therein.

S20.04: Data-based methods & learning

Date: March 20, 2024 14:00–16:00
Room: G22/122
Chair(s): Philipp, Friedrich
Othmane, Amine

Data-based methods for control: Why and how to incorporate machine learning

Bieker, Katharina
LMU München

14:00

With the exponential increase in available data and the growing accessibility to these resources, interest in data-driven methods and machine learning has surged across various technical and scientific domains, including control theory. Data-driven control methods allow for controlling complex and high-dimensional dynamic systems often better, more efficiently, robustly, and flexibly than traditional control methods or for initially learning and analyzing their system dynamics via system identification.

In this presentation, we first consider concrete applications and the resulting challenges that have to be taken into account when applying machine learning methods. At the core of the showcased approaches is the combination of model predictive control with machine learning for system identification. We particularly address how these methods contribute to reliability aspects, such as error bounds, safety guarantees, or interpretability. Different methods for identifying system dynamics will

be explored, and the proposed approaches will be illustrated and verified through numerical examples.

High Gain Observer Design for Nonlinear Systems using Machine Learning
Fiedler, Julius; Gerbet, Daniel; Röbenack, Klaus 14:40
TU Dresden

Neural networks are widely used for nonlinear pattern recognition and regression. A common type of neural network, the multilayer perceptron, can be trained to approximate the behavior of a function using input-output data of said function.

The control of dynamical systems usually relies on the knowledge of the internal state of the system. Typically, one is not able to measure all state components directly, which is why observers are employed to reconstruct the entire state from a measured output trajectory of the system. The concept of high gain observers is a well-established design method to estimate the state of a nonlinear system. Such observers are based on the transformation into the observability canonical form. It might be necessary, to embed the original system (dimension n) into a space of higher dimension (N) than the original.

Even though algebraic approaches for calculating the observability canonical form exist, they usually require large symbolic terms, that might lead to numerical problems. In our approach, we try to approximate the nonlinear maps required for calculating the normal form by training a neural network. E.g. the inverse transformation from the embedded state to the original state might be difficult to compute and evaluate, especially for N > n. Additionally we use automatic differentiation to avoid symbolic calculation during the embedding transformation.

Partial observations, coarse graining and equivariance in Koopman operator theory for large-scale dynamical systems
Peitz, Sebastian (1); Harder, Hans (1); Nüske, Feliks (2); Philipp, Friedrich (3); Schaller, Manuel (3); Worthmann, Karl (3) 15:00
1: Paderborn University
2: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
3: TU Ilmenau

The Koopman operator has become an essential tool for data-driven analysis, prediction and control of complex systems, the main reason being the enormous potential of identifying linear function space representations of nonlinear dynamics from measurements. Until now, the situation where for large-scale systems, we (i) only have access to partial observations (i.e., measurements, as is very common for experimental data) or (ii) deliberately perform coarse graining (for efficiency reasons) has not been treated to its full extent. In this talk, we address the pitfall associated with this situation, that the classical EDMD algorithm does not automatically provide a Koopman operator approximation for the underlying system if we do not carefully select the number of observables. Moreover, we show that symmetries in the system dynamics can be carried over to the Koopman operator, which allows us to massively increase the model efficiency. We also briefly draw a connection to domain decomposition techniques for partial differential equations and present numerical evidence using the Kuramoto–Sivashinsky equation.

Online learning with joint state and model estimation
Götte, Ricarda-Samantha; Timmermann, Julia 15:20
Paderborn University

Model-based state observers require high-quality models to deliver accurate state estimates. However, due to time or cost shortage, modeling simplifications or numerical issues models often have severe inaccuracies that may lead to insufficient and deficient control. Instead of attempting to iteratively model these deviations, we address the challenge by the concept of joint estimation [1]. Thus, we assume a linear combination of suitable functions to approximate the inaccuracies. The parameters of the linear combination are supposed to be time invariant and augment the model's state.

Subsequently, the parameters can be identified simultaneously to the states within the observer. Referring to the principle of Occam's Razor, the parameters are claimed to be sparse. Our former work [2,3] shows that estimating states and model inaccuracies simultaneously by a sparsity promoting unscented Kalman filter yields not only high accuracy but also provides interpretable representations of underlying inaccuracies.

Based on this work, our contribution is twofold: First, we apply our approach finally on a real-world test bench, namely a golf robot. Within the experimental setting, we investigate open and closed loop behavior as well as how suitable functions need to be chosen to approximate the inaccuracies in a physically interpretable way. Results do not only provide high state estimation accuracy but also meaningful insights into the system's inaccuracies.

Second, we discuss and establish a method to automatically adapt and update the model based on collected data of the linear combination during operation. Examining past parameter estimates by principal component analysis, a moving window is utilized to extract the most dominant functions. These are kept characterizing the model inaccuracies, while non-dominant functions are automatically neglected and refilled with novel function candidates. After analysis and rebuilding, this updated function set is subsequently fed back into the joint estimation loop and deployed for further estimation. Hence, we give a holistic paradigm of how to analyze and combat model inaccuracies while ensuring high state estimation accuracy. Within this setting, we once more investigate open and closed loop behavior and yield promising results.

In conclusion, we show that the proposed strategy provides a helpful tool to guarantee high estimation accuracy for models with severe inaccuracies or situations with occurring deviations during operation, e.g., due to mechanical wear or temperature changes.

Adaptive Data-Driven Models in Port-Hamiltonian Form for Control Design

Junker, Annika; Timmermann, Julia; Trächtler, Ansgar 15:40
Paderborn University

Control engineering applications usually require a model that accurately represents the generally nonlinear dynamics of the system. In addition to classical physical modeling, powerful data-driven approaches are gaining popularity. However, the resulting models may not be ideal for control design due to their black box structure and thus a lack of interpretability. In control engineering, formulating the system dynamics in PCHD form (Port-Controlled Hamiltonian Systems with Dissipation) [Mov00] is highly beneficial as the valuable property of being passive enables the straightforward design of globally stable controllers while ensuring physical interpretability. In a recently published article, we presented a method for data-driven inference of PCHD models for complex mechatronic systems, requiring only fundamental physical prior knowledge [JTT22]. The resulting models accurately represent the nonlinear dynamics of the considered system and are physical interpretable by incorporating the underlying physical principle of energy conservation.

In this contribution, we advance our previous work by including two key elements. Firstly, we demonstrate the application of the above described data-driven PCHD models for controller design. Preserving the PCHD form in the closed loop not only guarantees global stability and robustness but also achieves desired speed and damping characteristics [OvME02]. Since control systems continuously measure the state variables during operation due to the feedback structure, we secondly aim to use this data. Thus, we augment the existing modeling strategy with an intelligent adaptation approach to address (un)predictable system changes in mechatronic systems over the lifecycle, e.g., the installation of a new component, wear or temperature fluctuations during operation. Our proposed algorithm for a recursively calculated data-driven PCHD model utilizes a least-squares approach with extensions such as automatically adjusting the forgetting factor and controlling the covariance matrix trace. We showcase the results through model-based application on an academic example and experimental validation on a test bench.

[MOv00] Maschke, B. M.; Ortega, R.; van der Schaft, A. J.: Energy-based Lyapunov functions for forced Hamiltonian systems with dissipation. IEEE Transactions on Automatic Control, (45)8, 2000, S. 1498–1502

[JTT22] Junker, A.; Timmermann, J.; Trächtler, A.: Learning Data-Driven PCHD Models for Control Engineering Applications. IFAC-PapersOnLine, (55)12, 2022, S. 389–394*

[OvME02] Ortega, R.; van der Schaft, A.; Maschke, B.; Escobar, G.: Interconnection and damping assignment passivity-based control of port-controlled Hamiltonian systems. Automatica, (38)4, 2002, S. 585–596

S20.05: Data-based methods & learning

Date: March 20, 2024 16:30–18:30
Room: G22/122
Chair(s): Bieker, Katharina
Lanza, Lukas

Learning-based robust funnel MPC

Berger, Thomas (1); Dennstädt, Dario (1,2); Lanza, Lukas (2); Worthmann, Karl (2) 16:30
1: Paderborn University
2: TU Ilmenau

Model Predictive Control (MPC) is nowadays a widely used control technique relying on the iterative prediction of the future system behavior and solution of optimal control problems. Utilizing a particular stage cost design mimicking ideas from the adaptive model-free funnel control, the novel concept *funnel MPC* allows guaranteed output tracking of smooth reference signals with prescribed performance for non-linear multi-input multi-output systems. With ensured initial and recursive feasibility, this control objective is achieved without imposing any terminal conditions or requirements on the length of the prediction horizon. In this talk we present the most recent advances on *robust funnel MPC*, a two component control scheme directly combining the model-based funnel MPC with the model-free funnel control as an outer feedback-loop. This controller design results in a robust MPC algorithm and allows for the application of funnel MPC in the presence of unknown disturbances and even a structural plant-model mismatch. Extending the robust funnel MPC control scheme further by a learning component allows to continually adapt the underlying model to the system data and thereby improve the prediction capability required in MPC and the overall controller performance. The combined three component controller maintains predefined guarantees on the evolution of the tracking error while the learning component is able to perform safe online learning - even without an initial model or offline training.

Safe data-driven power grid synchronization

Lanza, Lukas; Schmitz, Philipp 16:50
TU Ilmenau

The use of system data in control mechanisms has attracted a lot of attention in recent years. Based on the seminal work [1] many results on data-enabled predictive control were developed recently. Following these developments, a data-driven predictive control algorithm for stabilization of the grid frequency of a power grid modeled via DAEs was proposed in [2]. Solely relying on input-output measurement data from the system, this controller successfully stabilizes the grid's utility frequency while respecting power demands. Although this controller shows good results, neither estimates nor guarantees for the stabilization are available.
To address the latter, in this contribution we extend the data-driven controller [2] by an additional feedback loop similar to [3]. The feedback controller is inherently robust and achieves stabilization within predefined performance margins. However, the control signal is computed online, thus, the output guarantees come to the cost of potentially rapidly changing control signals. We combine data-driven predictive control and pure feedback control to benefit from both: ahead-in-time prediction and stability guarantees. The effectiveness of the two-component controller is demonstrated by numerical simulations of energy grid stabilization.

[1] Willems, L. C., Rapisarda, P., Markovsky, I., and De Moor, B. L. M. (2005). A note on persistency of excitation. *Systems & Control Letters*, 54(4):325-329.

[2] **Schmitz, P**., Engelmann, A., Faulwasser, T., and Worthmann, K. (2022). Data-driven MPC of descriptor systems: A case study for power networks. *IFAC-PapersOnline*, 55(30):359-364. 25th International Symposium on Mathematical Theory of Networks and Systems MTNS 2022.
[3] **Schmitz**,**P**.,**Lanza, L.**, Worthmann, K. (2023). Safe data-driven reference tracking with prescribed performance. *27th International Conference on System Theory, Control and Computing (ICSTCC)*, 454-460.

The tangential AAA algorithm for learning MIMO-DAE dynamical systems from frequency-domain data

Benner, Peter; Gosea, Ion Victor; Heiland, Jan; Saak, Jens 17:10
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

The Adaptive Antoulas-Anderson (AAA) algorithm [1] is an effective approach to find a realization of a dynamical system from frequency response data (measurements of the system's transfer function). It efficiently blends interpolation and least squares fit, producing reliable and fast results. In the proposed work, we intend to devise an extension of AAA that is tailored to learning MIMO (multi-input multi-output) linear dynamical systems with DAE (differential-algebraic equation) terms. To accomplish this, we combine the tAAA (tangential AAA) approach in [2] with the results of the work in [3], that proposes a correction to the classical barycentric form used in AAA in order to account for the polynomial terms in the transfer function. The application of interest, amongst others, will be a linearized Navier-Stokes model with a significant non-proper behavior.

[1] Y. Nakatsukasa, O. Séte, L. N. Trefethen: The AAA algorithm for rational approximation, SIAM Journal on Scientific Computing, 40(3), A1494–A1522, 2018, DOI: 10.1137/16M1106122.

[2] Q. Aumann, P. Benner, I. V. Gosea, J. Saak, J. Vettermann: A tangential interpolation framework for the AAA algorithm, PAMM, e202300183, 2023, DOI: 10.1002/pamm.202300183.

[3] I. V. Gosea, J. Heiland: Implicit and explicit matching of non-proper transfer functions in the Loewner framework, submitted to the 22nd European Control Conference, 2023, available online at: https://arxiv.org/abs/2311.05519

Unveiling the Promise of Event Cameras for Underwater Robotics Localization for Agile Navigation

Alvarez-Tunon, Olaya (1); Alff, Thies Lennart (2); Bauschmann, Nathalie (2); Amer, Abdelhakim (1); Pham, Huy (1); Duecker, Daniel A. (3); Seifried, Robert (2); Kayacan, Erdal (4) 17:30
1: Aarhus University
2: Hamburg University of Technology
3: Technical University of Munich
4: Paderborn University

Event cameras revolutionize computer vision with their high temporal resolution and low latency. In robotics, particularly underwater robotics, the utilization of event cameras for localization remains largely unexplored although it is still one of the main challenges in navigation and control of autonomous underwater vehicles. The underwater environment presents unique challenges, including limited visibility, complex lighting conditions, and the high presence of dynamic elements such as marine snow. The potential benefits of event cameras should be exploited to address these challenges.

The present study conducts simulative and experimental evaluation of event-based localization. The research aims to compare several state-of-the-art event-based localization algorithms in underwater environments.

The state-of-the-art event-based methods implemented comprise EVO [1], ESVO [2], and EventEmin [3], which have proven outstanding performance in applications with high-speed motion scenarios. Furthermore, the ORB-SLAM3 and DSO algorithms are also implemented to compare the challenges and opportunities of event-based versus traditional state-of-the-art methods.

The simulated environments used are the ones introduced in [4]. These environments propose underwater pipeline inspection scenarios with different light levels and dynamic elements that challenge traditional computer vision algorithms.

By simulating various scenarios and conditions, the study provided insights into the performance of these algorithms and their adaptability to the challenges posed by underwater navigation.

The findings of the simulative study are encouraging, suggesting that event cameras hold promise for localization applications in underwater environments. The high temporal resolution and low-latency nature of event cameras proved beneficial in navigating the complexities of underwater settings. However, further experimentation and real-world testing are necessary to validate these simulation-based results and fully comprehend the advantages event cameras can offer to underwater robotics. Therefore, in a first step, experimental results performed in a confined water tank are presented.

In conclusion, the integration of event cameras into SLAM algorithms shows great potential for revolutionizing the field of robotics, particularly in challenging environments like underwater scenarios.

[1] Rebecq, H., et. al. (2016). Evo: A geometric approach to event-based 6-dof parallel tracking and mapping in real time. IEEE RAL, 2(2), 593-600.

[2] Zhou, Y., et. al. (2021). Event-based stereo visual odometry. IEEE Transactions on Robotics, 37(5), 1433-1450.

[3] Nunes, U. M., et. al. (2021). Robust event-based vision model estimation by dispersion minimisation. IEEE Transactions on Pattern Analysis and Machine Intelligence, 44(12), 9561-9573.

[4] O. Álvarez-Tuñón, et al., "MIMIR-UW: A multipurpose synthetic dataset for underwater navigation and inspection," *2023 IEEE/RSJ International Conference on Intelligent Robots and Systems.*

Possibilistic Robot Localization Using Visual Landmarks

Könecke, Tom; Ebel, Henrik; Hanss, Michael 17:50
University of Stuttgart

In robotics, the task of precisely and robustly locating mobile robots in their operating environments presents a significant challenge. While it is often technically feasible to achieve localization precision in the sub-millimeter range using high-end motion capture systems, a more cost-effective and easy-to-deploy approach that is less dependent on the accuracy of sensors is highly desirable. The idea is to compensate for the sensing inaccuracy by the robustness of the approach, i.e., its ability to deal with incomplete and imprecise data.
This contribution introduces an innovative camera-based localization approach for custom-built omnidirectional mobile robots, employing a fisheye lens to capture images toward the ceiling and horizon. Landmarks with known positions, in this case red poles, are positioned across the lab. By detecting these landmarks in the images, an estimate of the robot's position and orientation is made.
Several challenges arise from this setup. First, ambiguity stems from the fact that the robot's position is not always uniquely determined by its orientation with respect to a handful of indistinguishable landmarks. Furthermore, the live camera feed of a non-stabilized moving camera is often noisy and blurred, which can lead to landmarks not being detected in every frame.
The use of possibility theory as a theory of imprecise probabilities provides a robust framework for incorporating both the inherent ambiguity of the experimental setup as well as the uncertainties stemming from the image processing in dynamic state estimation. Furthermore, the use of possibility theory enables a connection to probabilistic confidence intervals by employing a calibration method using the aforementioned motion capture system as ground truth. This leads to a robust, rather than maximally accurate, localization method. It diverges from traditional single-point estimates, considering a distribution of possible robot positions across the entire state space, always incorporating only the available information. This inherent robustness may be particularly valuable for safety-critical applications, e.g., for robot collision avoidance.
The ability to dynamically give an uncertain state estimate of a system allows for the integration with a previously developed possibilistic filter algorithm where early results promise a significant improvement in the time-dependent state estimation of the robot.
In conclusion, this contribution demonstrates a novel approach for camera-based mobile robot localization and is another proof of concept for possibility theory bringing actionable insights to a real-world application.

These insights may lay the groundwork for future enhancements in uncertainty quantification for localization, particularly in dealing with incomplete and imprecise data.

Reversible methods in deep learning

Maslovskaya, Sofya (1); Ober-Blöbaum, Sina (1); Offen, Christian (1); Singh, Pranav (2); Wembe, Boris (1)

1: Paderborn University
2: University of Bath, UK

18:10

Deep learning is widely used in practical data analysis. It was shown to be especially successful in such tasks as image recognition and generation, in learning dynamical systems from data and more. Many applications require safety in learning and therefore it is important to develop theoretically based architectures. There has been considerable progress in this direction lately, where one of the approaches is to look at deep learning through the lens of dynamical systems. The propagation through layers in deep learning mimics numerical flow of a control system, where the control must be optimal to fit the data. This permits the use of methods from control theory and numerical analysis to design new architectures. It was recently shown that the combination of reversible discretizations together with the calculation of the gradients using the adjoint method lead to considerable reduction of the memory cost while computing correct gradients. On the other hand, it was shown that higher order methods are more accurate in the learning tasks related to dynamical systems. Only lower order reversible methods applicable to deep learning being known, it is important to also construct higher order methods. In this work we construct two classes of higher order reversible methods based on splitting and show their efficiency in examples.

S20.06: Nonlinear control

Date: March 21, 2024 08:30–10:30
Room: G22/122
Chair(s): Berger, Thomas
Heiland, Jan

Funnel MPC for nonlinear systems with arbitrary relative degree

Berger, Thomas; Dennstädt, Dario

Paderborn University

08:30

MPC is a well-established control technique which relies on the iterative solution of optimal control problems (OCPs). Recently, funnel-like ideas were introduced to overcome some limitations in MPC. The latter means that "artificial" assumptions are imposed to find an initially feasible solution and to ensure recursive feasibility of MPC (i.e., solvability of the OCP at a particular time instant automatically implies solvability of the OCP at the successor time instant). It was shown that these assumptions are superfluous when "funnel-like" stage costs are introduced so that the costs grow unbounded when the tracking error approaches the funnel boundary. More precisely, in contrast to simply adding the constraints on the tracking error to the OCP with standard quadratic stage costs, funnel MPC is initially and recursively feasible, without imposing state constraints or terminal conditions and independent of the length of the prediction horizon. Earlier results show this for a class of nonlinear systems with relative degree one or for systems with higher relative degree, but only in the presence of so called feasibility constraints. In this talk, we present a new approach where these limitations are avoided.

Model complexity optimization of equivalent dynamical linearization data models used in model-free adaptive control based on bias/variance trade-off

Salighe, Soheil; Söffker, Dirk 08:50
University of Duisburg-Essen

This paper discusses a strategy for optimizing the complexity of time-varying data models as used in model-free adaptive control (MFAC). Here the dynamic linearization in compact form (CFDL), partial form (PFDL), and full form (FFDL) are considered as equivalent data models used to describe input/output (I/O) data sets. These data models are built only for control purpose and can have various degrees of complexity depending on the size of the considered time-window. The methodology is to compare the performance of the data models according to an evaluation criterion, analyze the order of different data models based on bias/variance trade-off, and select the best performing data model. The complexity of the selected data model is compared with reduced LTI linear model obtained by applying a combination of eigensystem realization algorithm (ERA) and observer/Kalman filter identification (OKID) on the same set of I/O data. The I/O data is obtained from applying the MFAC controllers on a nonlinear three tank system (3TS) to track various desired references. The results indicate that the model complexity optimization can also be used for selecting an appropriate MFAC data model with optimal order to reduce the complexity and computational burden of the MFAC control algorithms.

Systematic Parameter Study on Joint Level Impedance Control - Towards a Variable Impedance Control Scheme for Legged Robots

Pérez Paz, Abelardo; Kist, Arian; Rixen, Daniel 09:10
Technical University of Munich

This contribution reports on an early investigation of joint level impedance control for use in legged robots. A methodology is presented to efficiently perform high resolution evaluations of various controller designs using a model of the robotic joint in question. The fundamental appeal of legged robots is their inheritance of the physical environmental adaptations that shaped humans and animals, whose bodies are laid out to deal with rugged terrain, unpredictable and frequently changing environments. Humans, in essence, move and balance by varying the impedance of their muscles through the degree to which they are contracted. Variable impedance control (VIC) uses the same principle, and is particularly attractive for legged robots due to these biomimetic properties. In this contribution, a model of a generic rotary robotic joint will be derived using system identification methods on a test rig. The test rig replicates a joint module from the humanoid robot LOLA developed at the Chair of Applied Mechanics of the Technical University of Munich. Impedance control relies on an inner torque control loop, realizing the torque demanded by the impedance relation as a function of the position deviation from the reference trajectory. The performance of various different torque control loop designs embedded within an impedance controller is evaluated in simulation using the previously derived mathematical model of the joint, saving testing time on hardware, sparing the test rig from repeated, demanding tests, and making tests that surpass the capabilities of the hardware but are interesting from a controller performance standpoint, possible in the first place. These evaluations contemplate how well a given controller can track a desired position and an impedance of choice. They cover the range of stable impedances for every controller, thereby helping the control system designer to evaluate tradeoffs like that between robustness and performance in the range of impedances relevant to the task at hand. With variable impedance control becoming more popular in impedance control applications, developing an understanding of how much parameters may vary before the system becomes unstable or performance becomes unacceptable is a crucial step in the development of an impedance controller.

Dual Quaternion parametrization of a Sliding Mode Control with Artificial Potential Functions

Stankovic, Ana; Müller, Wolfgang H. 09:30
TU Berlin

It has long been known that in the context of rotations, quaternions simplify the description of an object's orientation in three-dimensional space. The subject of this paper addresses the parameterization in dual quaternions, which can simultaneously describe the translation and rotation of a rigid body. While the representation of the motion equation is not a new insight, it leads to elegant equations that are incorporated into the paper to implement real control for a specific application.

Describing both rotation and translation simultaneously becomes particularly important when one wants to specify the exact positions of objects relative to each other. This is often the case in scenarios such as rendezvous and docking in space exploration. For this reason, the paper investigates the attitude control in close proximity operations of satellites.

As robust control is crucial for mission success, a Sliding Mode Control with Artificial Potential Functions is parameterized in dual quaternions for a simulation environment. The local minima problem of the Artificial Potential Functions is addressed in an application-specific manner, and additional constraints, such as field of view and collision avoidance, are considered.

The implementations are carried out in an Experimental Lab for Proximity Operations and Space Situational Awareness (ELISSA) simulation environment developed by TU Braunschweig. The paper contributes to the advancement of active debris removal measures, where it is necessary for the satellite to dock with tumbling space debris. Simulation scenarios are selected based on this application to evaluate the performance of the Sliding Mode Control with Artificial Potential Functions.

Design of Two Coupled Fuzzy Controllers for a Planar Direct Internal Reforming Solid Oxide Fuel Cell

Zhai, Tianyu; Bestle, Dieter 09:50
BTU Cottbus-Senftenberg

In the context of generating clean energy, fuel cells have a wide variety of applications from use as power unit in vehicles to decentralized stationary power generation. A special class is the direct internal reforming solid oxide fuel cell (DIR-SOFC) which may internally transform input methane into hydrogen, and which can absorb waste heat generated by electrochemical reactions. This can not only increase the efficiency but also affect the operating temperature of such fuel cells.

At first, a lumped dynamic model of a planar DIR-SOFC will be presented which involves a set of differential and algebraic equations resulting from species, mass and energy conservation laws as well as electrochemical reaction equations [1]. Simulation results regarding output voltage, power and temperature are analyzed in detail.

The second focus of this paper is on control of this model. During the operation of a DIR-SOFC the output power has to meet the demanded load, the working voltage has to stay always above the minimal design value, and the outlet cell temperature has to be kept at a specific design value in order to avoid thermal stress which would reduce service life of the DIR-SOFC. In order to achieve these goals, two independent fuzzy controllers are designed and coupled with the present nonlinear, time-variant DIR-SOFC model. The first controller accounts for the first two goals. It has two input signals which are the error between demanded and output power as well as the output voltage of the DIR-SOFC model. The second controller shall keep the temperature constant. For the latter, two different approaches are proposed: the first receives only the error between set value and outlet cell temperature as input signal, while the second also receives the time derivative of the outlet cell temperature.

Suitable choices of membership functions for fuzzification of input signals, base rules for control decisions and defuzzification approaches for the control outputs are defined and discussed. The control outputs are the inlet fuel flowrate for the first controller and the air flowrate for the second

controller, respectively. These flowrates are imported into the DIR-SOFC model as inputs to realize closed-loop control. Based on the simulation results, the two variants of the second controller are discussed.

[1] Huang, B., Qi, Y., Murshed, A.M: Dynamic Modelling and Predictive Control in Solid Oxide Fuel Cells: First Principle and Data-Based Approaches. Chichester: Wiley & Sons, 2012.

A two-step order reduction approach of incompressible Navier-Stokes equations for H-infinity robust nonlinear controller design

Heiland, Jan (1); Das, Amritam (2)
1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: Eindhoven University of Technology

10:10

The control of general nonlinear large-scale dynamical models is a challenging task. The computational challenges in the controller design come from both the possibly large state space and the nonlinear dynamics. In this work [1] we propose a two-folded model reduction approach tailored to nonlinear controller design for incompressible Navier-Stokes equations and similar PDE models that come with quadratic nonlinearities.

In a first step, we embed the nonlinear model in the class of linear-parameter varying (LPV) systems and then approximate only the parametrization on a very low dimensional manifold. This way, we obtain an approximation as an LPV system for which we can call on established controller design approaches and routines [2].

Since the computation of solutions to the involved linear matrix inequalities (LMIs) is not yet well suited for large scale systems, in a second step, we reduce the state-space dimension of the LPV approximation. With independent choices of the dimensions of state and parametrization, we can balance the complexity in the nonlinearity (should be rather small) and the state (can be of larger size for better accuracy).

We illustrate the procedure and discuss the computational challenges and its potentials in numerical simulations.

References

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[2]: Apkarian, P.; Gahinet, P., and Becker, G. Self-scheduled H-infinity control of linear parameter-varying systems: a design example (1995), Automatica(31), https://doi.org/10.1016/0005-1098(95)00038-X

S20.07: Control of distributed-parameter systems

Date: March 21, 2024 14:00–16:00
Room: G22/122
Chair(s): Röbenack, Klaus
Irscheid, Abdurrahman

Boundary control of distributed-parameter systems: A solution-based approach

Irscheid, Abdurrahman
Saarland University

14:00

The last two decades have witnessed a surge in research targeted towards boundary control of distributed-parameter systems. To a large degree, this can be traced to the development of the backstepping method for linear hyperbolic and parabolic partial differential equations (PDEs) with boundary actuation [3]. It was generalized to encompass dynamical boundary conditions, which yield PDEs that are bidirectionally coupled with ordinary differential equations (ODEs), denoted as PDE-ODE systems. Despite the success of backstepping in the linear case, it has yet to overcome the challenges associated with nonlinearities. Whilst a number of alternative methods have emerged for nonlinear hyperbolic systems, results for the parabolic case remain to be scarce.

This talk introduces a unifying framework for boundary control of nonlinear PDE-ODE systems in the context of the so-called solution-based approach [2, 1]. Interestingly, solution-based designs can be viewed as an extension of backstepping due to the equivalence of both methods for linear systems. The presentation puts forth an intuitive perspective to provide a general understanding of the main ideas with a focus on benchmark examples. In particular, the method relies on the solution of a suitable Cauchy problem; a concept also relevant for flatness-based open-loop control [4]. As such, for implementing the control law, an efficient numerical scheme is suggested to solve these problems online. The performance of the proposed approach is demonstrated in simulative studies.

References

[1] A. Irscheid, N. Gehring, J. Deutscher, and J. Rudolph. Solution-based control: An extension of backstepping for nonlinear parabolic PDE-ODE systems. Under review.
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[3] M. Krstic and A. Smyshlyaev. Boundary Control of PDEs: A Course on Backstepping Designs. SIAM, 2008.
[4] J. Rudolph. Flatness Based Control of Distributed Parameter Systems. Shaker Verlag, 2003.

Control design for convection-reaction systems with storage effects and positive relative degree

Wurm, Jens; Woittennek, Frank 14:40
Private University for Health Sciences and Health Technology (UMIT Tirol), Austria

One dimensional distributed parameter systems consisting of several convection-reaction equations, which are distributed coupled with a reaction equation are considered. These models can be used, for example, to model thermal pipe flow, desalination plants, or the kinetic behaviour of catalysts in large gas engines. In typical applications, the outflow of one of the convection-reaction systems is to be transferred between stationary regimes, with an inflow variable serving as the control input. The remaining variables are considered known disturbances. To solve the resulting open-loop control problem an inversion based approach is proposed. Along the common characteristics projection the system can be reduced to a single partial differential equation the boundary conditions of which result from the particular choice of the output to be tracked. The solution of this latter equation constitutes the basis of the control design.

The particular properties of the scalar boundary value problem to be solved depend on the coupling structure of the originally given convection-reaction system. While in most cases, the output possesses relative degree 0, for practical applications relative degree 1 is of particular interest. In this case, the obtained scalar boundary value problem which describes the internal dynamics, possesses the structure of a non-regular infinite dimensional differential-algebraic equation (DAE). Within the talk, the properties of the solution of this DAE are discussed from both an analytical system theoretic point of view, and a numerical point of view. Apart from the open-loop design which is able to account for known disturbances, a closed-loop output-tracking scheme can be deduced from the solution of the DAE. For the original model, which has been written on the characteristics for the above described analysis, this scheme results in a predictor based feedback. The contribution discusses the proposed scheme for a selective catalytic reduction (SCR) catalyst.

Open-Loop Control of Shallow Water Waves in a Tube with Moving Boundary in Material-Fixed Coordinates

Mayer, Luca; Woittennek, Frank 15:00
Private University for Health Sciences and Health Technology (UMIT Tirol), Austria

The well-known Saint-Venant equations are often used to model shallow water in open channels, such as irrigation channels with rectangular cross-sections [1–3]. Another application of the shallow water equations is the modeling of snow avalanches [4, 5]. This contribution focuses on the open-loop control design for the system addressed in [6–10] - specifically, a one-dimensional shallow water model with moving boundary and arbitrary cross section. To account for the time-varying spatial domain,

the model equations as well as the control design are formulated and considered in material-fixed coordinates. Within this framework, emphasis is placed on achieving smooth transitions between stationary regimes, in particular ensuring that the water level at the unactuated boundary follows a predefined trajectory. This trajectory corresponds to the transition of the flat output between two steady states. It is important to emphasize that, despite the change to material-fixed coordinates, the procedure for designing the open-loop control is very similar to that used in Eulerian coordinates (cf. [8]). Therefore, the shallow water equations are linked as boundary value problems, transformed into hyperbolic normal form and solved using the method of characteristics. With this solution, complete parameterization of the control input through the flat output allows the planned transition to be realized.

In order to simulate the considered system and to validate the planned trajectory, the numerical models derived in [6, 7] are used. These models are based on an appropriate discretization of the original spatially distributed model. To preserve the stability properties of the original model during the approximation, energy-based methods are particularly suitable. In [6], the underlying model was transformed from Eulerian (spatially-fixed) to Lagrangian (material-fixed) coordinates and spatially discretized in an energy-preserving manner. This methodology was further extended to higher-order approximation methods in [7], where the resulting energy-preserving semi-discrete models were simulated at low resolution.

Trajectory tracking control based on computer vision of a two-way soft prototype actuated with SMA wires

Acevedo-Velazquez, Aline Iobana; Wang, Zhenbi; Winkler, Anja; Modler, Niels; Röbenack, Klaus
TU Dresden
15:20

This research focuses on achieving precise trajectory tracking of the deformation angle of a 3D-printed soft prototype manufactured with thermoplastic polyurethane (TPU) and actuated with shape memory alloy (SMA) wires, by using a controller based on a computer vision system that analyzes the deformation of the soft prototype in real-time.

The computer vision system consists of a camera that captures the soft prototype, then using image processing algorithms the visual information is transformed into the variable of deflection angle. Then, this deflection angle is sent to the controller which calculates the proper voltage needed for the soft prototype so that it follows predefined trajectories with accuracy.

To achieve precise trajectory tracking, a control system with feedback and feedforward is implemented. The feedforward signal uses the nominal model of the prototype and the trajectory information to calculate a control signal. The feedback control, on the other hand, utilizes the actual data obtained by the camera in real-time to adjust the deflection angle and guarantee that the tracking error is reduced. It can be shown that the addition of a feedforward term to the feedback controller enhances the performance.

Feedback semiglobal stabilization to trajectories for the Kuramoto–Sivashinsky equation

Seifu, Dagmawi Abraham
Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria
15:40

It is shown that an oblique projection based feedback control is able to stabilize the state of the Kuramoto–Sivashinsky equation, evolving in rectangular domains, to a given time-dependent trajectory. The actuators consist of a finite number of indicator functions supported in small subdomains. Simulations are presented, in the one-dimensional case under periodic boundary conditions and in

the two-dimensional case under Neumann boundary conditions, showing the stabilizing performance of the feedback control.

S20.08: System analysis

Date: March 21, 2024 17:40–18:40
Room: G22/122
Chair(s): Yevgenieva, Yevgeniia
Gerbet, Daniel

On the Kolmogorov n-width of reachable sets of the bilinear Schrödinger equation

Zuyev, Alexander; Feng, Lihong; Benner, Peter 17:40
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

We consider the problem of approximating the reachable sets by finite-dimensional linear varieties for a class of nonlinear distributed-parameter control systems. This problem is studied within the framework of the Kolmogorov n-width of sets in a Banach space. Analytical estimates of the n-width of the image of a given set under the action of a bounded nonlinear operator are proposed. These estimates are applied to the analysis of the endpoint map associated with the bilinear Schrödinger equation with a scalar input. We characterize the n-width of the corresponding reachable set, depending on the control constraints on a given finite time interval.

Well-posedness and exponential stability of a controlled dispersed flow tubular reactor model

Yevgenieva, Yevgeniia; Zuyev, Alexander; Benner, Peter 18:00
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

We study a mathematical model of n^{th}-order chemical reactions of the type "A $\rightarrow$product" carried out in a dispersed flow tubular reactor (DFTR). The reactor dynamics is governed by a nonlinear parabolic partial differential equation with boundary data controlled by a single input, as described in [1]. The well-posedness of the corresponding nonlinear Cauchy problem is proved within the framework of strongly continuous semigroups of operators and perturbation theory. It is shown that the considered model admits an equilibrium corresponding to a constant input. In the current work, we focus on the analysis of the qualitative behavior of trajectories in a neighborhood of this equilibrium. The exponential stability of the steady state is established within Lyapunov's direct method. Further extension of this approach towards obtaining polynomial decay rate estimates is discussed.

[1] Petkovska, M., Seidel-Morgenstern, A.: Evaluation of periodic processes, in the book by Silveston, P.L., Hudgins, R.R., Eds.: Periodic Operation of Chemical Reactors, Butterworth-Heinemann, Oxford (2013), Chapter 14, 387-413.

Towards checking BIBO stability for hyperbolic systems

Wierzba, Alexander A. 18:20
University of Twente, The Netherlands

In this contribution we consider aspects of Bounded-input-bounded-output (BIBO) stability for systems described by infinite-dimensional linear state-space representations. In this setting subtleties not present in the finite-dimensional case arise. A focus is placed on systems with boundary control and observation, in particular towards characterizing necessary and sufficient conditions for the class of port-Hamiltonian systems.

S20.09: Model order reduction

Date: March 22, 2024 08:30–10:30
Room: G22/122
Chair(s): Mehrmann, Volker
Gosea, Ion Victor

Structure-Preserving Interpolation of Quadratic-Bilinear Systems via Regular Multivariate Transfer Functions

Benner, Peter (1,2); Gugercin, Serkan (3); Werner, Steffen W. R. (3) 08:30
1: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
2: Otto von Guericke University Magdeburg
3: Virginia Tech, USA

For accurate modeling of real-world phenomena, high-dimensional nonlinear dynamical systems are indispensable. Thereby, many physical properties are encoded in the internal differential structure of these systems. Some examples for differential structures are second-order time derivatives in mechanical systems and time-delay terms. When using such models in computational settings such as in numerical simulations, the high-dimensional nature of the models represented by large numbers of differential equations describing the dynamics becomes the main computational bottleneck. A remedy to this problem is model order reduction, which is concerned with the construction of cheap-to-evaluate surrogate models that are described by a significantly smaller number of differential equations while accurately approximating the input-to-output behavior of the original high-dimensional system. It has been shown that many nonlinear phenomena can be equivalently modeled using quadratic-bilinear systems. Therefore, many established model order reduction approaches such as transfer function interpolation and balanced truncation have been extended to the class of quadratic-bilinear systems in recent years. However, in most cases, these approaches cannot be applied to systems with internal differential structures. In this work, we present a structure-preserving interpolation framework for the regular multivariate transfer functions of quadratic-bilinear systems. This new approach allows the simulation-free construction of reduced-order models for quadratic-bilinear systems with internal structures and it is able to preserve differential structures in the reduced-order model.

Extending balanced truncation to general domains

Borghi, Alessandro (1); Breiten, Tobias (1); Gugercin, Serkan (2) 08:50
1: TU Berlin
2: Virginia Tech, USA

Model order reduction aims to alleviate the computational burden of large-scale systems by computing a lower order surrogate model with approximately the same input-output behaviour. While many established techniques exist in this field, a substantial amount assumes the underlying model to be asymptotically stable.

The objective of this work is to extend existing methodologies to linear time invariant systems with transfer functions having poles in more general domains in the complex plane.
In particular, we generalize the concept of balanced truncation, a widely adopted model reduction technique. To this aim, we reformulate the Gramians of the full order system. We demonstrate that, under certain assumptions, these Gramians are the solution to Lyapunov equations. Lastly, we show that there exists a bound for a newly defined H2 norm.
We propose a balanced-truncation-based algorithm and assess its performance against systems with poles on the imaginary axis.

Optimization-based model order reduction of port-Hamiltonian descriptor systems

Schwerdtner, Paul (1); Moser, Tim (2); Mehrmann, Volker (3); Voigt, Matthias (4) 09:10
1: New York University, USA
2: Technical University of Munich
3: TU Berlin
4: UniDistance Suisse, Switzerland

We present a new optimization-based structure-preserving model order reduction (MOR) method for port-Hamiltonian differential-algebraic equations (pH-DAEs). Our method is based on a novel parameterization that allows us to representany linear time-invariant pH-DAE of a prescribed model

order. We propose two algorithms which directly optimize the parameters of a reduced model to approximate a given large-scale model with respect to either the H∞or the H2 norm.This approach has several benefits. Our parameterization ensures that the reduced model is again a pH-DAE system and enables a compact representation of the algebraic part of the large-scale model, which in projection-based methods often require a more involved treatment. The direct optimization is entirely based on transfer function evaluations ofthe large-scale model and is therefore independent of the structure of the system matrices. Numerical experiments are conducted to illustrate the high accuracy and small reduced model orders in comparison to other structure-preserving MOR methods.

Model reduction of descriptor systems with quadratic output functionals

Przybilla, Jennifer; Pontes Duff, Igor; Goyal, Pawan; Benner, Peter
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

09:30

This work is dedicated to the model reduction of differential-algebraic systems with quadratic output (`DAE_QO`) functionals of the form

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \qquad x(0) = 0, \\ y(t) &= x(t)^T M x(t). \end{aligned}$$

Under some mild conditions, these systems can be transformed into a Weierstraß canonical form and thus decouple into a differential equation and an algebraic equation and the corresponding differential and algebraic states.
In contrast to the case of differential-algebraic systems with linear output (`DAE_LO`), the system `DAE_QO` presents a coupling of the differential and algebraic states in the output signal. Our goal is to determine the dominant subspaces of the differential and algebraic states and reduce the system accordingly.
To this end, we propose new Gramians that encode the suitable subspaces and we demonstrate their relationship with energy functions. Firstly, we show that reachability is encoded by the proper and improper reachability Gramians, similarly to the `DAE_LO` case. For the observability, we decompose the system output into four subsystems, two of those associated with differential states and the other two with algebraic states.
Based on this subsystem decomposition, we derive new observability Gramians for the differential and algebraic state vectors. They can be determined by solving continuous-time and discrete-time Lyapunov equations.
Finally, the proper reachability and observability Gramians are then used to derive a reduced differential state space using balanced truncation.
Additionally, the improper Gramians are used to truncate uncontrollable and unobservable algebraic states.
Furthermore, we derive an error estimator which is used to evaluate the quality of the reduced surrogate model. Finally, we illustrate the effectiveness of our method by applying it to example problems.

Model Order Reduction for switched Differential Algebraic Equations

Manucci, Mattia; Unger, Benjamin
University of Stuttgart

09:50

In this presentation, we will discuss a projection-based Model Order Reduction (MOR) for large-scale systems of switched Differential Algebraic Equations (sDAEs). The main idea relies on exploiting the Quasi-Weierstrass form of each mode of the sDAEs system. Then, we can show that, under certain reasonable assumptions, the output of the sDAEs system is equivalent to the output of a switched system of ordinary differential equations (ODEs) with state jumps between the modes. We present how to construct a reduced system by computing the controllability and observability Gramians associated with the solution of generalized Lyapunov equations for bilinear systems. Finally, we discuss how to efficiently compute an approximation of the solution of such generalized Lyapunov equations, with error control, when the associated matrices are sparse and large.

Numerical results are presented to showcase the efficiency and effectiveness of the developed MOR method.

Removing Inconsistencies of Reduced Bases in Parametric Model Order Reduction by Matrix Interpolation

Schopper, Sebastian; Müller, Gerhard
Technical University of Munich

10:10

Simulations of complex, parametric, dynamical systems using the Finite Element Method can become computationally very expensive since large systems of equations have to be solved for multiple instances in time or frequency and for a wide range of parameters. To reduce the numerical effort of one simulation, projection-based model order reduction (MOR) methods can be used. Here, the system is projected onto a lower dimensional subspace that contains the desired solution. To retain the parametric dependency in the reduced-order model, Parametric MOR can be used. Many of those methods require an affine representation of the parametric dependency, which is difficult to realize for e.g., geometric parameters.

Parametric MOR based on matrix interpolation does not require such affine parametric dependency. In this method, local reduced models are first computed for a set of samples in the parameter space. Afterwards, the local reduced bases are transformed such that they align as close as possible with a generalized coordinate system. If all local reduced-order models are described in a similar coordinate system after the transformation, an interpolation of the reduced operators can be performed to obtain the solution for queried parameter points with little computational effort. However, the transformation is not possible if the reduced bases for different samples span different subspaces. This can happen due to mode switching and truncation of some of those modes in the reduction, but also due to inherent changes of the reduced bases with the change of the parameters. Both reasons introduce inconsistencies in the training data for the matrix interpolation. Consequently, the predicted reduced-order models are not accurate.

In this work, adaptive sampling is used in combination with partitioning of the parameter space into subdomains to ensure consistent reduced bases. In the first step, the subspace angles between the local reduced bases of neighboring samples are computed. If the largest subspace angle is below a user-defined threshold, the two reduced bases are consistent; if it is around 90°, the two bases are inconsistent. For a subspace angle between the two thresholds, a new sample is required in between to find out, whether the samples are consistent or not. This procedure is repeated until the reduced bases of all neighboring samples are known to be either consistent or inconsistent with each other. Finally, the parameter space is partitioned between samples with inconsistent bases to obtain subdomains, within which all local reduced bases are consistent with each other.

S21: Mathematical signal and image processing

Organizer(s): Wald, Anne *(University of Göttingen)*
Maly, Johannes *(Ludwig-Maximilians-Universität München)*

S21.01: Mathematical Signal and Image Processing (Part I)

Date: March 19, 2024 08:30–10:30
Room: G22/208
Chair(s): Wald, Anne
Maly, Johannes

Virtual X-rays: parallel-beam tomography hidden within electric probing

Siltanen, Samuli 08:30
University of Helsinki, Finland

X-ray tomography (CT) and Electrical Impedance Tomography (EIT) are two fundamental inverse problems. CT is based on recording X-ray data of the patient along several angles of view. Image reconstruction is geometrically straightforward, linear, and only mildly ill-posed. However, as a downside the patient is exposed to ionising radiation.
In EIT, the patient is probed with harmless electric currents, and the resulting voltages are measured. The mathematical model of EIT is the inverse conductivity problem [Calderón 1980]. The currents travel along curved paths, determined by the unknown conductivity distribution, so image reconstruction in EIT is nonlinear. Moreover, EIT is very ill-posed, demanding a high level of regularization against measurement noise and modelling errors.
A fundamental connection between EIT and CT was found in [Greenleaf et al. 2018] by using microlocal analysis. There, it was shown that a one-dimensional Fourier transform applied to the spectral parameter of Complex Geometric Optics (CGO) solutions produces virtual X-ray projections, enabling a novel filtered back-projection type nonlinear reconstruction algorithm for EIT. Note that there are no actual X-rays; the measurements are current-to-voltage data collected with electrodes.
The above analysis paves the way for a novel decomposition of the EIT inverse problem. It turns out that all ill-posedness of EIT can be confined into two linear steps in the decomposition. The other one is classical Radon inversion of parallel-beam CT and thus only mildly ill-posed. The other is a collection of one-dimensional deconvolutions with a known Gaussian kernel (a third fundamental inverse problems appears!), which is highly ill-posed. The new approach to EIT, called Virtual Hybrid Parallel Tomography (VHPT), offers unprecedented reconstruction strategies for EIT, including maximally interpretable ways of including machine learning to sub-problems.
The first real-data images by VHPT are presented, and implications to medical imaging and process monitoring are discussed.

Denoising of Sphere- and SO(3)-valued Data by Relaxed Tikhonov Regularization

Beinert, Robert; Bresch, Jonas; Steidl, Gabriele 09:10
TU Berlin

Manifold-valued signal- and image processing has received attention due to novel image acquisition techniques. Recently, a convex relaxation of the Tikhonov-regularized nonconvex problem for denoising circle-valued data has been proposed by Condat (2022) using positive semidefinite matrices. Based on Schur complement arguments, we show that this variational model can be simplified while leading to the same solution. Our simplified model can be generalized to higher dimensional spheres and to SO(3)-valued data, where we rely on the quaternion representation of the later one. Standard algorithms from convex analysis can be applied to solve the resulting convex minimization problem. As proof-of-the-concept, we use the alternating direction method of minimizers to demonstrate the denoising behavior of the proposed method in the context of hue and cromaticity denoising.

Accelerating 3D Topology Optimization through Sample-Efficient Deep Learning

Erzmann, David (1); Dittmer, Sören (1,2)
1: University of Bremen
2: University of Cambridge

09:30

Recent developments in Deep Learning show great potential for density-based Topology Optimization. However, this subfield still faces challenges due to a lack of established methods and datasets. We propose a novel approach to address these issues by integrating physics-based preprocessing and equivariant neural networks into an efficient Deep Learning pipeline. We demonstrate significant improvements in sample efficiency and physical correctness of predictions. Finally, we address one of the primary bottlenecks in Topology Optimization by showcasing the application of Neural Operators as substitutes for classical Partial Differential Equation solvers.

Postprocessing U-Net for the Kuopio Tomography Challenge 2023

Denker, Alexander (1); Freudenberg, Tom (1); Kluth, Tobias (1); Kereta, Zeljko (2); Singh, Imraj (2); Arridge, Simon (2)
1: University of Bremen
2: University College London

09:50

The Finish Inverse Problem Society organized the Kuopio Tomography Challenge 2023 (KTC2023), a competition focused electrical impedance tomography (EIT) reconstruction techniques under limited data conditions. Our contribution, securing a position in the Top 3, involves the implementation of a postprocessing U-Net approach trained exclusively on a simulated dataset.

EIT aims to reconstruct the distribution of conductivity within an object's interior based on voltage measurements obtained from its boundary. The challenge, comprising 7 progressively complex levels, required participants to address limited-view reconstruction scenarios by successively removing boundary electrodes.

Our submission introduces a novel postprocessing U-Net designed to directly predict the conductivity map using an initial reconstruction and the challenge level as input. The initial reconstruction leverages linearized difference reconstruction, incorporating NOSER, the graph Laplacian, and a smoothness prior for regularization. The training of our postprocessing U-Net involved a dataset of synthetic phantoms and simulated measurements.

S21.02: Mathematical Signal and Image Processing (Part II)

Date: March 19, 2024 16:30–18:30
Room: G22/208
Chair(s): Wald, Anne
Maly, Johannes

Data driven enhanced methods in terahertz tomography including a partially learned Landweber iteration

Schuster, Thomas; Meiser, Clemens
Saarland University

16:30

We consider the inverse problem of terahertz tomography which is an imaging technique for monitoring plastics and ceramics. The underlying mathematical problem is associated with Maxwell's equations and simplifications thereof. Starting with the non-linear eikonal equation as a physical model, we address this challenge by the Landweber iteration respecting the theory of inverse problems. The eikonal equation results as a high frequency approximation of the Helmholtz equation and, more generally, of the wave equation. Our primary task is to deduce the refractive index, denoted as n(x), from time-of-flight measurements.
In a second step, we introduce neural networks in the Landweber iteration for the reconstruction of the refractive index n(x). Applying Landweber's method, we have to solve the non-linear partial differential equation for the forward operator for each initial condition in every step but also need to

compute the adjoint operator of the Fréchet derivative. To reduce the computing time in the reconstruction process, we substitute the forward operator F by a Convolutional Neural Network. Using synthetic training data which consist of the refractive index and simulated measure data, we accelerate significantly the evaluation of the forward operator, i.e., the solution of the eikonal equation, compared to standard techniques such as marching schemes. Furthermore, we save energy in the learning process of our network by generating a sparse forward operator. We add to the cost functional of the Convolutional Neural Network an l_1-regularization term. We then compare the standard Landweber method with the partially learned and the sparse alternative, presenting our numerical results.
Additionally, we develop and implement a data driven anomaly detection algorithm for in-line monitoring with a particular focus on plastics. We propose a density-based approach to automatically detect anomalies in the radiation's measured data. We will also illustrate numerical results to support our findings. The real measured values are provided by the German Plastics Center (SKZ) in Würzburg. This is joint work with Clemens Meiser from Saarland University Saarbrücken.

Using feasibility constraints in the data space do deal with unknown rigid motion in (Nano-)CT

Ehlers, Björn; Wald, Anne; Lucht, Jens; Salditt, Tim 16:50
University of Göttingen

In computerized tomography (CT) the measurement process can be modeled using the Radon transform, which maps the unknown material density to the corresponding absorption loss.
In Nano-CT the scale is so small that vibrations of the measuring apparatus lead to unwanted rigid movement of the scanned object. This motion is also unknown, so it can not easily be incorporated in a model.
Using then the inexact model, which assumes no motion, will lead to artefacts. These artifacts occur because the measured data, which would need to be modeled with movement and detector noise, is not in the range of the assumed operator. However, this fact can be utilised, if there is only a small intersection of the range, from the assumed motionless operator, and the motion-set, which contains all the possible data for the possible rigid motions of the object.
In this talk we will present some ways to approximate this motion-set with a convex set, using multiple measurements, sinogram interpolation and data consistency conditions.
In the reconstruction we then can use the convex sets as feasibility constraint in the data space using the Chambolle-Pock method.

Real data EIT reconstruction using virtual X-rays and deep learning

Rautio, Siiri (1); Alsaker, Melody (2); Moura, Fernando (3); Agnelli, Juan Pablo (4); Murthy, Rashmi (5); Mueller, Jennifer (6); Lassas, Matti (1); Siltanen, Samuli (1) 17:10
1: University of Helsinki, Finland
2: Gonzaga University, USA
3: Federal University of ABC, Brazil
4: National University of Cordoba, Argentina
5: Bangalore University, India
6: Colorado State University, USA

We introduce a new reconstruction algorithm for electrical impedance tomography, which provides a connection between EIT and traditional X-ray tomography, based on the idea of "virtual X-rays". We divide the exponentially ill-posed and nonlinear inverse problem of EIT into separate steps. We start by mathematically calculating so-called virtual X-ray projection data from the measurement data. Then we perform explicit algebraic operations and one-dimensional integration, ending up with a blurry and nonlinearly transformed Radon sinogram. We use neural networks to remove the higher-order scattering terms and perform deconvolution. Finally, we can compute a reconstruction of the conductivity using the inverse Radon transform. We demonstrate the method with experimental data.

Reconstruction of active forces generated by actomyosin networks

Klass, Emily; Wald, Anne
University of Göttingen

17:30

Biological cells rely on the interaction of proteins to perform various forms of movement such as cell contraction, division, and migration. In particular, the proteins actin is able to create long branching filament structures which the protein myosin can bind to and slide along on. These acto-myosin networks produce mechanical stress resulting in movement in the inside of the cell that can lead to self-propulsion.

We aim to reconstruct the active forces inside of the droplet from noisy measurements of the velocity field. This results in a (deterministic) parameter identification problem for the Stokes equation.

We depict the physical process of the flow inside of such cells generated by acto-myosin networks using a 2-dimensional droplet model with the Stokes equation for incompressible Newtonian fluids for non-constant viscosities. Here we add a Neumann boundary condition where the normal component of the velocity field on the boundary of the droplet vanishes to represent that no fluid can flow in or out of the domain. Further, we add a Robyn-type or slip boundary condition to model the interaction with surrounding fluids. We choose a non-constant viscosity to portray the acto-myosin network.

Motion Correction in Fluorescence Microscopy

Beutler, Sascha (1); Kunisch, Manuel (2); Pilger, Christian (2); Huser, Thomas (2); Wirth, Benedikt (1)
1: University of Münster
2: Bielefeld University

17:50

In living organisms the natural motion caused e.g. by the heartbeat, breathing, or muscle movement leads to the deformation of tissue due to stretching and displacement.
This causes the plane of observation to shift or deform in intravital imaging experiments, which limits the observation time for specific points of interest.
In this talk the mathematical idea of how to determine the three-dimensional, time-dependent deformation from two-dimensional sectional images is presented.
Given this deformation the future position of the points of interest can be rapidly calculated and the point of interest can be observed for a longer time at high imaging frame rates and without the need for mechanical tissue fixation.

S21.03: Mathematical Signal and Image Processing (Part III)

Date: March 20, 2024 08:30–09:30
Room: G22/208
Chair(s): Maly, Johannes
Wald, Anne

Differential Prony-Type Method for Approximation of the Gaussians

Derevianko, Nadiia
University of Göttingen

08:30

We propose a differential Prony-type method to approximate the Gaussian function on the real line by a short exponential sum. We prove that the optimal frequency parameters for our method in the weighted L_2 approximation problem are zeros of a scaled Hermite polynomial. This observation leads us to a numerically stable approximation method with low computational cost. Furthermore, we derive a direct algorithm to solve this approximation problem based on a matrix pencil method for a special structured matrix. The entries of this matrix are determined by hypergeometric functions. For the weighted L_2-norm, we prove that the approximation error decays exponentially with respect to the length N of the sum. The talk is based on joint research with Gerlind Plonka (University of Göttingen).

Fourier-Domain Inversion for the Modulo Radon Transform
Beckmann, Matthias
University of Bremen
08:50

Inspired by the multiple-exposure approach in computational photography, recently, several practitioners have explored the idea of high dynamic range (HDR) X-ray imaging and tomography to deal with high intensity projections that exceed the dynamic range of the detector. While establishing promising results, these approaches inherit the limitations of the multiple-exposure fusion strategy. To overcome these disadvantages, in our recent line of work the modulo Radon transform has been proposed, which is based on a co-design of hardware and algorithms. In the hardware step, Radon transform projections are folded using a modulo non-linearities to avoid sensor saturation. Thereon, recovery is performed by algorithmically inverting the folding, thus enabling a single-shot, HDR approach to tomography.
In this talk we propose a novel Fourier-domain recovery algorithm that is based on the Orthogonal Matching Pursuit (OMP) algorithm as well as the non-equispaced Fast Fourier Transform (NFFT). The advantages of OMP-NFFT include recovery at lower sampling rates while being agnostic to the modulo threshold, lower computational complexity and empirical robustness to system noise. Beyond numerical simulations, we use prototype modulo ADC based hardware experiments to validate our claims, where we report image recovery based on hardware measurements up to 10 times larger than the sensor's dynamic range while benefiting with lower quantization noise.
This talk is based on joint work with Ayush Bhandari (Imperial College London) and Meira Iske (University of Bremen).

THE INFORMATION GEOMETRY OF SMART
Raus, Maren (1); Elshiaty, Yara (1); Petra, Stefania (2)
1: Heidelberg University
2: University of Augsburg
09:10

We investigate the problem of minimizing Kullback-Leibler divergence between a linear model Ax and a positive vector b in different domains (e.g. positive orthant, n-dimensional box, probability simplex). Our focus is on the SMART (Simultaneous Multiplicative Algebraic Reconstruction Technique) method, that employs efficient multiplicative updates. We explore the exponentiated gradient method, which can be viewed as a Bregman proximal method and a Riemannian gradient descent on the parameter manifold of a corresponding exponential family. This dual interpretation enables us to establish connections and achieve accelerated SMART iterates while smoothly incorporating constraints.

S21.04: Mathematical Signal and Image Processing (Part IV)
Date: March 20, 2024 14:00–16:00
Room: G22/208
Chair(s): Maly, Johannes
Wald, Anne

Algorithmic regularization in asymmetric overparameterized matrix sensing
Soltanolkotabi, Mahdi (2); Stöger, Dominik (1); Xie, Changzhi (2)
1: Katholische Universität Eichstätt-Ingolstadt (KU)
2: University of Southern California
14:00

There has been significant progress in understanding the convergence and generalization properties of gradient-based methods for training overparameterized learning models. However, many aspects including the role of small random initialization and how the various parameters of the model are coupled during gradient-based updates to facilitate good generalization remain largely mysterious. In this talk, we consider a general overparameterized low-rank matrix sensing problem where one wishes to reconstruct an asymmetric rectangular low-rank matrix from a few linear measurements. We show that in this setting, factorized gradient descent enjoys an algorithmic regularization property where the iterates show a propensity towards low-rank models despite the overparameterized nature

of the factorized model. This allows us to show that the gradient descent trajectory from small random initialization moves towards solutions that are both globally optimal and generalize well.

Unraveling Acoustic Signal Patterns in Fisheries Through DINO-Based Self-Supervised Learning

Pala, Ahmet (1); Oleynik, Anna (1); Malde, Ketil (2); Handegard, Nils Olav (2)

1: University of Bergen, Norway
2: Institute of Marine Research, Norway

14:20

Acoustic surveys provide important data for fisheries management. During the surveys, ship-mounted echo sounders send acoustic signals into the water and measure the strength of the reflection, so-called backscatter. Acoustic data, the collection of those backscatters, are annotated by manual processes which are resource-intensive and time-consuming. In addition, during these annotation processes, only target fish species are typically labeled, leaving other structures such as zooplankton layers unlabeled. Recently introduced supervised methods help with the annotation process. Those methods, however, still rely on the annotations which are incomplete and hard to get.

Our main objective in this research is to develop a robust and annotation-free methodology to advance the analysis of fisheries acoustic data. We use the self-supervised method based on DINO (Self-Distillation with No Labels) which was introduced for computer vision tasks. The DINO model learns image representations from global and local views of the image and creates the corresponding feature embeddings that can be used for subsequent tasks. This is achieved using two networks, a teacher and a student, with the same network architecture. They generate normalized K-dimensional features using temperature SoftMax and are compared through cross-entropy loss. Gradients flow only through the student network, and the teacher's parameters are updated using an exponential moving average of the student's parameters.

We have systematically adapted the DINO model to handle acoustic data by substituting images with fixed-sized acoustic patches. Additionally, we have refined data augmentation techniques to align with the unique characteristics of acoustic data. The resulting embeddings were then analyzed using a basic k-NN algorithm, utilizing pre-existing labels. The classification algorithm resulted in a high precision of patch classification. Additionally, when clustering the embeddings corresponding to the unlabeled portion of the acoustic data, distinct structures within the data were observed to form cohesive clusters. This implies that the self-supervised method can identify unique energy patterns in different regions of the acoustic data and could be used to assist with acoustic data exploration and annotations.

Our findings highlight the importance of emerging self-supervised techniques in the signal processing domain, specifically for acoustic data in fisheries research. This methodology fills the research gap of self-supervised learning application in the fisheries acoustics domain from a mathematical signal and image processing viewpoint.

Comparing the Performance of Beamformer Algorithms in Estimating Orientations of Neural Sources

Buschermöhle, Yvonne (1,3); Höltershinken, Malte Bernhard (1,2); Erdbrügger, Tim (1,2); Radecke, Jan-Ole (4,5); Sprenger, Andreas (5,6,7); Schneider, Till (8); Lencer, Rebekka (4,5); Gross, Joachim (1,3); Wolters, Carsten (1,3)

1: Institute for Biomagnetism and Biosignalanalysis, University of Münster
2: Institute for Analysis and Numerics, University of Münster
3: Otto Creutzfeldt Center for Cognitive and Behavioral Neuroscience, University of Münster
4: Department of Psychiatry and Psychotherapy, University of Lübeck
5: Center of Brain, Behaviour and Metabolism, University of Lübeck
6: Department of Neurology, University of Lübeck
7: Institute of Psychology II, University of Lübeck
8: Department of Neurophysiology and Pathophysiology, University Medical Center Hamburg-Eppendorf

14:40

An accurate reconstruction of both the location and orientation of neural activity is a critical component of many neuroscientific and medical applications. Examples include epilepsy diagnosis, where information about the generators of epileptic activity can be inferred from source reconstructions, or electric brain stimulation, where the efficacy crucially depends on the injected current being aligned with the orientation of the targeted neuronal population. Using EEG and MEG source analysis, we can derive source estimates using non-invasive measurements of electric potentials and magnetic fluxes at the head surface. One inverse method of particular interest is beamforming, which has been shown to accurately estimate source activity even in the presence of high noise and interfering signals. While a lot of research focuses on beamformer performance for source localization, i.e. the estimation of the position of neural activity, analyses on assessing the accuracy of beamforming-based orientation estimation are still lacking. In this work, we contribute to the latter, by examining the theoretical properties of the common beamformer algorithms in idealized settings. Furthermore, we compare, in simulation studies, the performance of the beamformer algorithms for different signal-to-noise ratios, and for different modalities. Specifically, we investigate the Unit-Gain (UG), Array-Gain (AG), and Unit-Noise-Gain (UNG) beamformer algorithms, and prove that AG and UNG beamformers have no bias in the orientation estimation, independent of the noise level. Meanwhile, the UG beamformer introduces a noise-dependent bias into the estimation. Furthermore, we show that the combined EEG/MEG orientation estimation can outperform the pure EEG estimation, depending on the signal-to-noise ratio of the single modalities.

S22: Scientific computing

Organizer(s): Walther, Andrea *(Humboldt-Universität zu Berlin)*
Hesch, Christian *(University of Siegen)*

S22.01: Various topics in Scientific computing

Date: March 19, 2024 08:30–10:30
Room: G22/120
Chair(s): Stoll, Martin

Model Reduction of Hamiltonian systems: From the formulation on manifolds to data-driven realizations

Buchfink, Patrick (2); Glas, Silke (1); Haasdonk, Bernard (2); Mu, Hongliang (1); Unger, Benjamin (2)
1: University of Twente, The Netherlands
2: University of Stuttgart

08:30

In this talk, we present structure-preserving model reduction of Hamiltonian systems with nonlinear projections for problems with slowly decaying Kolmogorov-n-widths. In particular, we focus on the preservation of structure in the reduced order model (ROM) since otherwise the reduced model can be unreliable. In order to highlight the quantities that we would like to retain, we start by a formulation of the Hamiltonian system on manifolds. Beginning with this formulation, we derive a ROM on an embedded submanifold and then provide data-driven ansatzes how to realize this reduction method. In the numerical experiments, we demonstrate the ability of the methods to achieve a higher accuracy than structure-preserving linear-subspace ROMs.

Reducing the entry barrier of Peridynamic simulations

Hesse, Jan-Timo (1); Willberg, Christian (1); Pernatii, Anna (2)
1: German Aerospace Center (DLR)
2: Otto von Guericke University Magdeburg

09:10

Despite the broad applicability of Peridynamics, a persistent challenge remains: how to encourage widespread adoption. In the engineering domain, classical continuum mechanics, predominantly facilitated by the finite element method, enjoys extensive utilization, supported by a plethora of commercial and open-source software tools.
Peridynamic simulation tools often find themselves in competition with these well-established counterparts. In research, custom codes tailored for specific applications are frequently created and applied, with little consideration for their future reuse or third-party utilization. The complexity is further exacerbated in High-Performance Computing applications, where a deep understanding of solvers, parallel computing, and Peridynamic itself is imperative for a successful software development. Given the constraints of a typical doctoral thesis, large-scale problems are often left unexplored, and research tends to be confined to simplistic geometries.
This presentation aims to elucidate various pathways for the seamless integration and utilization of a Peridynamic framework. We will showcase examples that illustrate how the barriers for both users and developers can be significantly lowered. Performance tests of large scale problems and several functionalities, as well as their integration, will be presented. Based on this foundation, future coupling with Finite Element Method (FEM) will be undertaken. Therefore, the entire system is modular structured to allow further integration of numerical methods.

Gradient based optimization method for temporal multiscale differential problems

Chang Dominguez, Dayron; Richter, Thomas
Otto von Guericke University Magdeburg

09:30

Temporal multiscale problems, characterized by the manifestation of long-term effects influenced by periodic processes occurring at a much faster scale, pose significant computational challenges. Instances of such problems are widespread, ranging from material weathering and fracture due to

atomistic defects to the degradation of materials through physical-chemical interactions and biological growth processes. Full simulations of models representing these processes incur substantial computational costs, requiring the solution of the problem for each *fast* timescale until the desired long-term effect is achieved. Moreover, in order to fit their parameters, it is necessary to be able to execute hundreds of simulations, which is almost impractical if the full resolution of those problems has to be accomplished. Temporal multiscale methods, such as Heterogeneous Multiscale Methods (HHM) and Variational Multiscale Methods (VMM), leverage the inherent temporal multiscale structure and quasi-periodic behavior to reduce computational effort. These methods assume that *fast* variables have a very low effect in *slow* variables over a certain number of periods, enabling the fixation of the latests for computing quasi-periodic solutions. While these methods offer significant computational reductions, parameter fitting remains crucial. This talk introduces a new numerical method for computing the gradient with respect to the parameters of the problem. This method facilitates the use of a fitting technique based on gradient descent, specifically designed to align with the unique multiscale structure of the problem. This method addresses this challenge by deducing the derivatives with respect to time of the derivatives with respect to the parameters for the different scale functions separately. Doing so two Ordinary Differential Equation (ODE) systems for each scale are derived. The solution of these systems precisely yields the components of the gradient with respect to the parameters necessary as inputs for the fitting method. This method not only avoids the numerical errors that arise from applying finite differences to determine the gradient of such a problem but also leverages the features of multiscale method solvers. Moreover, it can be numerically computed alongside the multiscale solver, as it computes each step of the simulation. Consequently, at the conclusion of each simulation, it becomes feasible to obtain the desired gradient. This new approach not only improves computational efficiency in fitting temporal multiscale problems but also serves as a valuable tool for making research in problems with long-term effects more viable.

MESHFREE Simulations for Industrial Applications

Castelli, Fabian; Michel, Isabel; Kuhnert, Jörg
Fraunhofer ITWM

09:50

Numerical simulations have become an indispensable tool for industrial research and development processes. Despite recent advances in numerical methods, software and hardware, the simulation of industrial applications is computationally challenging.

Classical discretization methods, such as the finite element or finite volume method, are meshbased and face crucial challenges for example in case of complex model geometries, large deformations, or free surfaces. Meshfree approaches overcome the expensive meshing step for classical methods.

At Fraunhofer ITWM and Fraunhofer SCAI, we develop and implement the MESHFREE software (www.meshfree.eu) providing a simulation tool for industrial applications. The discretization is based on a Generalized Finite Difference Method (GFDM). The method is purely meshfree and suited for fluid as well as continuum mechanical processes. Due to its discretization based on a scattered set of numerical points, MESHFREE is flexible and particularly efficient for applications with moving geometric parts, free surfaces, phase boundaries, or fluid-structure interaction. Examples include water management of vehicles or metal cutting processes.

The talk presents the MESHFREE software and introduces the mathematical formulation as well as theory behind the GFDM. The capabilities of MESHFREE are demonstrated with an overview of successfully simulated industrial applications.

Robust matrix-free polynomial preconditioning using the hyper-power method

Mika, Michał Łukasz; ten Eikelder, Marco F. P.; Schillinger, Dominik; Hiemstra, Rene R.
TU Darmstadt

10:10

We explore the integration of the hyper-power sequence, a method commonly employed for approximating the Moore-Penrose inverse, to enhance the effectiveness of an existing preconditioner. The approach is closely related to polynomial preconditioning based on Neumann series. We commence with state-of-the-art matrix-free isogeometric preconditioners designed for elliptic problems

descretized by the Galerkin method. Our results demonstrate that incorporating multiple iterations of the hyper-power method enhances the effectiveness of the preconditioner, leading to a substantial reduction in both iteration counts and overall solution time. Through a comprehensive theoretical analysis, we assess the stability, accuracy, and numerical cost associated with the proposed scheme. Multiple benchmarks show robustness with respect to a wide range of model parameters and geometric mappings.

S22.02: Various topics in Scientific computing

Date: March 19, 2024 16:30–18:30
Room: G22/120
Chair(s): Glas, Silke

Identification of temperature-dependent material parameters in piezoelectricity

Kuess, Raphael; Jurgelucks, Benjamin; Walther, Andrea 16:30
Humboldt-Universität zu Berlin

Piezoelectric materials are virtually present in almost all electrical devices nowadays, being prevalent not only in households but also in industrial and medical settings. The versatility of piezoelectric materials extends across a diverse range of products, including electronic toothbrushes, microphones and ultrasonic imaging devices, as well as humidifiers and loudspeakers. In this context, the accurate characterization of the temperature-dependent behavior of these materials is crucial, as high precision is required in many applications, but the material data provided by the manufacturers often deviates significantly from the actual data and is difficult to measure.

Therefore, our focus is on the reliable identification of the temperature-dependent parameters in the underlying system of partial differential equations coupling the mechanical displacement and the electrical potential. Herein, we will discuss the forward operator of the inverse problem and linearize our parameter identification problem by discretization in the temperature domain. Finally, we will solve this inverse problem using appropriate optimization and regularization techniques.

Consequently, the central focus will be on modeling and solving the linearized inverse problem by fitting to simulated and measured data, where numerical examples will be given.

Optimal Dirichlet Boundary Control by Fourier Neural Operators Applied to Nonlinear Optics

Margenberg, Nils (1); Kärtner, Franz X. (2,3); Bause, Markus (1) 16:50
1: Helmut Schmidt University, University of the Federal Armed Forces Hamburg
2: Universität Hamburg
3: Helmholtz Imaging, Deutsches Elektronen-Synchrotron DESY

We present an approach for solving optimal Dirichlet boundary control problems of nonlinear optics by using deep learning [Margenberg, N., Kärtner, F. X., & Bause, M. (2023). Optimal Dirichlet Boundary Control by Fourier Neural Operators Applied to Nonlinear Optics. https://arxiv.org/abs/2307.07292]. For computing high resolution approximations of the solution to the nonlinear wave model, we propose higher order space-time finite element methods in combination with collocation techniques. Thereby, C^1-regularity in time of the global discrete solution is ensured. The simulation data is used to train solution operators that effectively leverage the higher regularity of the training data. The solution operator is represented by Fourier Neural Operators and can be used as the forward solver in the optimal Dirichlet boundary control problem.
The proposed algorithm is implemented and tested on high-performance computing platforms, with a focus on efficiency and scalability. The effectiveness of the approach is demonstrated on the problem of generating Terahertz radiation in periodically poled Lithium Niobate. The neural network is used as the solver in the optimal control setting to optimize the parametrization of the optical input pulse and maximize the yield of 0.3THz-frequency radiation.
We exploit the periodic layering of the crystal to design the neural networks. The networks are trained to learn the propagation through one period of the layers. The recursive application of the network onto itself yields an approximation to the full problem. Our results indicate that the proposed method

can achieve a speedup by a factor of 360 compared to classical methods. A comparison of our results to experimental data shows the potential to revolutionize the way we approach optimization problems in nonlinear optics.

Parameter Identification for a Two-Compartment Contrast Flow Field Model
Externbrink, Sophie; Ruprecht, Daniel; Götschel, Sebastian 17:10
Hamburg University of Technology

Tumor perfusion and vascular properties are important determinants of a cancer's response to therapy. Thus being able to derive those parameters from patient-specific data collected at the bedside would give the opportunity for a better, more individual tumor treatment. Here we consider 3D dynamic contrast-enhanced ultrasound measurements, where propagation of a contrast agent is measured to estimate perfusion.
Models describing the transport of contrast agent based on advection-diffusion equations are most commonly found, but they lack the ability to derive physically accurate solutions for the transportation of tracer through an organ. Therefor, Sourbron (IEEE Trans Med Imaging 33(4):935-46, 2014, doi: 10.1109/TMI.2014.2300450) proposed a two-compartment model, where each voxel contains an arterial and venous blood compartment and contrast can exchange from the arterial to the venous compartment. Thus the flow of contrast agent is modeled by separating the arterial and venous flows into a system of transport equations, coupled by a transfer coefficient function which describes the exchange speed of the contrast agent from arteries to veins through capillaries.
In this talk we discuss the parameter identification problem, i.e., how to estimate flow velocities and the conversion coefficient function, given the concentration of contrast agent over time. We derive adjoint equations for efficient gradient computation, discuss the discretization of state and adjoint equation as well as the use of Leray projection within the optimization algorithm to ensure a divergence free velocity field, and present numerical examples.

Data- and knowledge-constrained splines for the prediction of physical phenomena
Haag, Claudius; Keip, Marc-André; Fritzen, Felix 17:30
University of Stuttgart

We present a spline-based computational approach for the prediction of physical phenomena that integrates quantitative (discrete, data-based) and qualitative (axiomatic, feature-based) evidence and information.
For this approach, a new software-package for flexible spline-based regression is proposed: It enables to complement the available data by constraining the ansatz space by physical conditions.
While the former are obtained from observation and given quantitatively (but potentially suggested to uncertainty and noise), the latter can be incorporated qualitatively through explicit function and parameter constraints, wiggle-constraints [1] or general non-linear constraints.

As examples we consider three applications: First, a mechanical problem with partial unknowns is considered to solve an inverse problem. We reconstruct either the unknown cross-section area A(x) or Young's modulus E(x) from noisy samples of the displacement field.
Second, we apply our software toolchain to discrete and unknown statistical data in order to identify the best probability density function (PDF) and its parameters.
In this context we minimize the Kullback-Leibler divergence [2] of parameterized PDFs against our spline regressor.
Third, analytical expressions of instability landscapes [3] will be generated by least-squares minimization [4] taking into account both, numerically obtained datasets of instability points and a-priori known physical features. The effect of the latter is the possibility to rely on much scarcer datasets inducing pronounced computational savings.

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Isogeometric methods for the simulation of electric motors considering rotation

Merkel, Melina (1); Kapidani, Bernard (2); Vázquez, Rafael (3); Schöps, Sebastian (1)

1: TU Darmstadt
2: EPFL, Switzerland
3: University of Santiago de Compostela, Spain

17:50

Isogeometric analysis (IGA) is a method for the discretization and numerical solution of partial differential equations. In contrast to the classical finite element method, it uses the basis functions from computer-aided design (i.e. B-splines and NURBS) for the representation of both geometry and solution. Originally applied for the solution of mechanical problems IGA has recently gained popularity in different fields. When applying IGA for the simulation of electric machines, we are faced with several challenges, such as the need for gauging techniques, nonconformity of moving parts and the necessary discretization of the air. In this work we present methods for an isogeometric workflow to overcome these challenges. In the case of rotating machines, conformity of the patches cannot be guaranteed for all rotation angles without modification of the geometry. We therefore use domain decomposition methods, e.g., mortaring or Nitsche type coupling, for the coupling of stator and rotor.

This work is supported by the joint DFG/FWF Collaborative Research Centre CREATOR (CRC – TRR361/F90) and the Graduate School CE within the Centre for Computational Engineering at Technische Universität Darmstadt.

S22.03: Various topics in Scientific computing

Date: March 20, 2024 08:30–09:30
Room: G22/120
Chair(s): Walther, Andrea

Multiscale flow simulations of dilute polymeric solutions with bead-rod chains using Brownian configuration fields

Meier, Andreas (1); Bänsch, Eberhard (1); Frank, Florian (1,2)

1: FAU Erlangen-Nürnberg
2: Math2Market GmbH, Germany

08:30

Polymeric fluids are of non-Newtonian type as they show viscoelastic characteristics. The modeling of such fluids is often done with constitutive models or multiscale models, where kinetic theory is used for the description of the polymer dynamics on the microscale.

In this talk, we couple the Navier–Stokes equations with the microscopic freely jointed bead-rod chain model (Kramers chain) to simulate dilute polymeric fluids. The bead-rod chain model approximates polymers with beads that are connected by rods to enforce a constant distance between neighboring beads. In contrast to simpler low dimensional bead-spring models, the high dimensional bead-rod chain model introduces multiple additional challenges, due to explicit constant rod length constraints and high computational costs, which requires special care. For the discretization, we use the Brownian configuration field method combined with the finite element method. Due to the Monte–Carlo nature of the Brownian configuration field method, additional parallelization beyond domain partitioning is utilized. The coupling to the Navier–Stokes equations enables the consideration of complex flow scenarios, where the bead-rod chains can influence the underlying flow field, which is done for start-up shear flow and the flow around a cylinder scenario.

Experiences from the development of a hybrid reduced order stochastic/LES solver for turbulent flows

Marinković, Pavle; Schöps, Mark Simon; Medina Méndez, Juan A.; Klein, Marten; Schmidt, Heiko 08:50
BTU Cottbus-Senftenberg

In this work, we discuss recent experiences related to the development and enhancement of the existing Computational Fluid Dynamics (CFD) solver, the C++ version of the Implicit/Explicit (IMEX) time-advancement algorithm used in the One-Dimensional Turbulence-based (ODT) Large Eddy Simulation (LES) model, abbreviated as ODTLES [1]. After being ported from Fortran 90 using minimal object-oriented programming, the current capabilities of the C++ code are restricted to the reproducibility of turbulent channel flow simulations with respect to the former Fortran code version [1], which was able to achieve reasonable agreement with existing Direct Numerical Simulation (DNS) data for low to moderate Reynolds number turbulent channel flows [2]. This is far from a satisfactory standpoint, and current efforts are centered on improving the solver code structure through comprehensive refactoring, robust unit testing, and strict adherence to code style guides, following the principles advocated in [3]. Our goals and experience are shared by colleagues who have worked in other state of the art, high performance computing (HPC) codes [4]. We focus the discussion on a methodology to balance unit, regression and integration testing. Unit testing, specifically, is often overlooked in CFD codes, with many established platforms like OpenFOAM focusing more on integration testing. Preliminary results will focus on the testing of the LES component of the code. To that extent, besides unit testing, an integration test using the method of manufactured solutions will be considered [5]. Future work will enhance the component-based development in order to conveniently interchange the use of ODT in ODTLES by other turbulence models which could range from classical LES subgrid scale models, to other stochastic models such as HiPS [6]. Such model selection need not be static, rather, it could be a dynamic one, enabling the solver to study a broad spectrum of turbulent flow conditions by intelligently selecting the most adequate type of subgrid scale model for a given flow regime.

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Improving the convergence of pseudo-time stepping for CFD simulations with neural networks

Zandbergen, Anouk (1); Heinlein, Alexander (2); van Noorden, Tycho (3) 09:10
1: TU Berlin
2: TU Delft
3: COMSOL, Netherlands

Computational fluid dynamics (CFD) simulations of viscous fluids described by the Navier-Stokes equations are considered. The Navier-Stokes equations may exhibit a highly nonlinear behavior, depending on the Reynolds number. Discretization of the Navier-Stokes equations leads to a system of nonlinear equations, which can be solved using nonlinear iteration methods, such as Newton's method. However, to obtain fast quadratic convergence, the Newton iteration must be close enough to the solution. Resulting that, for many configurations, the classical Newton iteration does not converge at all, and so-called globalization techniques may help to improve convergence.

In this talk, pseudo-time stepping is employed as a globalization technique to improve convergence for the stationary Navier-Stokes equations. The classical algorithm is enhanced by a neural network

model trained to predict the local pseudo-time step. To facilitate generalization, the pseudo-time step will be predicted on element level using local information on a patch of adjacent elements as input for the network. Numerical results for standard benchmark problems, including flow through a backward facing step (BFS) geometry and Couette flow, are presented to show the performance of the machine learning-enhanced globalization technique.

S22.04: Various topics in Scientific computing

Date: March 20, 2024 14:00–16:00
Room: G22/120
Chair(s): Walther, Andrea

GPU Acceleration of a General Purpose Finite Element Framework

Kaya, Utku (1); Liebchen, Manuel (1); Lessig, Christian (2); Richter, Thomas (1)
1: Otto von Guericke University Magdeburg
2: European Centre for Medium-Range Weather Forecasts

14:00

GPUs are today available as accelerator hardware in almost all computers, from laptops and workstations to powerful supercomputers. Despite this, the use of these accelerators for finite element imulations has so far been limited. Reasons are the considerable effort to port code to the GPU and that their programming paradigm is difficult to exploit for adaptive finite element methods. As a result, a large part of the available computer power remains currently unused.

In this talk, we describe the use of GPUs in the linear solvers of the general purpose finite element library Gascoigne [1]. Gascoigne has a focus on complex multiphysics problems and is build around a geometric multigrid method that allows for an adaptive grid control based on quadtree and octree meshes. In our extension of Gascoigne, we targeted an implementation that is highly efficient but requires only minimal changes to the library and ensures code maintainability. For this purpose, all operations of the multigrid method as well as the treatment of locally refined grids with hanging nodes is based on matrix-vector multiplications. Porting to the GPU is then carried out using the cuSparse library with particular attention being paid to avoid memory transfers between the CPU and GPU.

As example, we present linear elasticity, a convection-diffusion problem, and the time-dependent Navier-Stokes equations. Our results show that the efficiency of the methods depends strongly on the formulation of the code based on matrix-vector products. This is a major limitation in the treatment of general nonlinear problems. Nevertheless, we will demonstrate for the Navier-Stokes equations that an acceleration by a factor of 15 can be achieved compared to multicore systems.

[1] https://gascoigne.math.uni-magdeburg.de/

Floating-point accuracy and symbolic spectral decomposition of 3x3 matrices

Zilian, Andreas; Habera, Michal
University of Luxembourg

14:20

Spectral decomposition of matrices is a fundamental and pivotal operation in applied mathematics, physics, and engineering. Many practical applications necessitate the examination of 3x3 matrices with spectral decomposition over the real number spectrum. If the functional dependence of the spectral decomposition on the matrix elements has to be preserved, then symbolic representations become imperative.

Existing closed-form expressions predominantly rely on principal matrix invariants, yet their application encounters shortcomings within the scope of finite precision arithmetic. This contribution presents an alternative method for computing key matrix invariants, specifically focusing on the discriminant, by employing sum-of-products expressions as functions of the matrix elements.

This alternative approach notably enhances floating-point accuracy, particularly in critical scenarios such as those involving eigenvalue multiplicity. Several applications to problems in mechanics in the context of automatic differentiation and code generation are presented.

Improving performance of the ICON-O ocean model using parallel spectral deferred corrections

Freese, Philip (1); Hoffmann, Lars (2); Kadow, Christopher (3); Korn, Peter (4); Lapolli, Fabricio (4); Lu, Yen-Sen (2); Ruprecht, Daniel (1); Witte, Maximilian (3)

1: Hamburg University of Technology
2: Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH
3: German Climate Computing Center
4: Max Planck Institute for Meteorology, Hamburg

14:40

As part of the ExaOcean project, we are aiming to improve the performance of the ICON-O ocean model using machine learning and parallel in time methods. For the latter, we intend to implement parallel spectral deferred corrections (SDC) as a new numerical time-stepping method tailored to improve performance on many-core CPUs.

In our talk, we focus on the example of the shallow water equation and first present a reformulation of the SDC using the optimized routines of the ICON code. Our results show the promising performance of this approach, indicating the potential to choose larger time steps without compromising stability. Furthermore, even in the sequential case, fewer computations are required to achieve the same level of accuracy as the currently used Adams-Bashforth 2 scheme. Finally, we turn to time parallelization, introducing the parallel SDC scheme, giving some insight into the implementation, and showing further results.

Low-rank Lyapunov ADI on the GPU

Schulze, Jonas; Saak, Jens

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

15:00

Continuous-time algebraic Lyapunov equations arise in the fields of, e.g., optimal control and model order reduction. For many applications, the coefficient matrices are large and sparse, while the solution matrix has a low numerical rank. In this setting, the alternating-directions implicit (ADI) method, which directly operates on the low-rank factors of the solution matrix, is one of the most widely used algorithms for this type of equation. So far, GPUs have only been used to accelerate an older formulation of the low-rank ADI which did not reduce the need of complex arithmetic. In this work, we report on our progress of using the GPU to accelerate the most-recent formulation of the (inexact) low-rank Lyapunov ADI, which is a stepping stone towards a mixed-precision implementation.

Multilevel Block Partitioning for Solving Sylvester-like Matrix Equations

Köhler, Martin

Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

15:20

Solving Sylvester-like matrix equations is still a core task in systems and control theory. Their solution is also required in the large field of eigenvalue analysis. In addition to numerous iterative algorithms, Bartels and Stewart presented an algorithm for dense matrices in the 1970s. This algorithm has been improved over the last two decades by introducing techniques such as recursive blocking, level-3 block partitioning, and task-based scheduling. In the 2010s, Köhler and Saak showed that early GPU accelerators provided only a negligible speedup. Today, the computing infrastructure has moved from multi-core to many-core systems, and accelerators offer higher floating-point performance, higher memory bandwidth, and much better interconnection between CPUs and GPUs. These fundamental changes in hardware require further steps to accelerate the Bartels-Stewart algorithm. On the one hand, the available parallelism on the CPU side requires hundreds of (small) tasks, as in task-based scheduling algorithms, to make the Bartels-Stewart algorithm run as fast as possible. On the other hand, accelerator devices such as GPUs require a critical problem size to become efficient. Since the required block size for a CPU task-based algorithm does not meet the requirements for fast GPU execution, we had to extend the existing algorithms. In this talk, we present an algorithm that combines the ideas of recursive blocking, level-3 partitioning, and task-based scheduling using the StarPU library as a hybrid scheduling library. By using multiple levels of block partitioning, we simultaneously satisfy the block size requirements for both CPU and GPU. The StarPU library then schedules the individual

tasks to the computing devices that are most likely to result in the minimum execution time. Numerical results show that we can reduce the runtime for solving a Lyapunov equation of order 20,000 from 43.29s, using a level-3 BLAS approach on the CPU, to 2.44s, using our new hybrid multi-level block partitioning CPU-GPU execution scheme.

Numerical realization of the Mortensen observer via a Hessian-augmented polynomial approximation of the value function

Breiten, Tobias (1); Kunisch, Karl (2,3); Schröder, Jesper (1) 15:40

1: TU Berlin
2: University of Graz
3: Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austria

Two related numerical schemes for the realization of the Mortensen observer or minimum energy estimator for the state reconstruction of non linear dynamical systems subject to deterministic disturbances are proposed and compared. Both approaches rely on a polynomial approximation of the value function associated with the energy of the disturbances of the system. Such an approximation is obtained via interpolation considering not only the values but also first and second order derivatives of the value function in a set of sampling points. The scheme is applied to four examples and the results are compared with the well known extended Kalman filter.

S23: Applied operator theory

Organizer(s): Hussein, Amru *(RPTU Kaiserslautern-Landau)*
Grothaus, Martin *(RPTU Kaiserslautern-Landau)*

S23.01: Applied Operator Theory 1

Date: March 21, 2024 08:30–10:30
Room: G22/112
Chair(s): Hussein, Amru
Grothaus, Martin

A spectral inclusion property of essential spectrum of operator pencils

Wilson, Mitsuru (1); Trunk, Carsten (1); Hassen, Khlif (2)
1: TU Ilmenau
2: University of Sfax, Tunisia

08:30

In this study, we consider a closed densely defined linear operator A and a bounded linear operator B on a Banach space X with essential spectrums that are contained in non-intersecting sectors. Our key result establishes that the essential spectrum of the associated operator pencil $\lambda A + B$ is contained within a sector of the complex plane. Notably, the boundaries of this sector are determined solely by the angles characterizing the sectors containing the essential spectrums of A and B. This finding provides valuable insights into the spectral behavior of the combined operator pencil, shedding light on the geometric relationships between the essential spectrums of the individual operators.

Spectrum of the Maxwell Equations for a Flat Interface between Homogeneous Dispersive Media

Dohnal, Tomas (1); Brown, Malcolm (2); Plum, Michael (3); Wood, Ian (4)
1: Martin Luther University Halle-Wittenberg
2: Cardiff University
3: Karlsruhe Institute of Technology
4: University of Kent

09:10

The study of time harmonic electromagnetic waves at the interface of dispersive (i.e. frequency dependent) media leads to a non-self-adjoint operator pencil with the spatial curl-curl operator and a complex valued dielectric constant ε. The generally complex nature is in order to allow for non-conservative media (e.g. metals). A classical application is to surface plasmon polaritons. We assume that the interface is located at x=0 and the media in the two half spaces are spatially homogenous. The dependence of εon the spectral parameter ω(frequency) is generally nonlinear and we make no assumptions on its form.
The whole spectrum consists of eigenvalues and the essential spectrum, but the various standard types of essential spectra do not coincide in all cases. The main tool for determining the essential spectra are Weyl sequences. The functional setting is such that the operator domain is not a subset of the range which brings about a difficulty in defining the discrete spectrum.

S23.02: Applied Operator Theory 2

Date: March 21, 2024 14:00–16:00
Room: G22/112
Chair(s): Grothaus, Martin
Hussein, Amru

Optimal Sobolev Regularity for Degenerate Equations of Porous Media Type

Gess, Benjamin (1,3); Sauer, Jonas (2) 14:00

1: Bielefeld University
2: Friedrich Schiller University Jena
3: Max Planck Institute for Mathematics in the Sciences, Leipzig

We consider solutions to nonlocal, nonlinear, degenerate equations of porous media type. In contrast to the classical porous medium equation, the linear operator can be of an integro-differential operator of pure jump type, and the nonlinearity does not have to be of pure power type. In this talk I explain how the method of kinetic formulation and averaging lemmas can be utilized to obtain (both in the local and nonlocal case) Sobolev regularity results that are in line with the optimal regularity suggested by scaling arguments and which are consistent with the limiting linear case.

The talk is based on joint work with Benjamin Gess.

Existence and Uniqueness of Solutions of the Koopman–von Neumann Equation on Bounded Domains

Stengl, Marian (1,2); Gelß, Patrick (1,3); Klus, Stefan (4); Pokutta, Sebastian (1,2) 14:40

1: Zuse Institute Berlin
2: TU Berlin
3: FU Berlin
4: Heriot-Watt University, Edinburgh

The Koopman–von Neumann equation describes the evolution of a complex-valued wavefunction corresponding to the probability distribution given by an associated classical Liouville equation. Typically, it is defined on the whole Euclidean space. The investigation of bounded domains, particularly in practical scenarios involving quantum-based simulations of dynamical systems, has received little attention so far. We consider the Koopman–von Neumann equation associated with an ordinary differential equation on a bounded domain whose trajectories are contained in the set's closure. Our main results are the construction of a strongly continuous semigroup together with the existence and uniqueness of solutions of the associated initial value problem. To this end, a functional-analytic framework connected to Sobolev spaces is proposed and analyzed. Moreover, the connection of the Koopman–von Neumann framework to transport equations is highlighted.

A Galerkin projection approach for general port-Hamiltonian descriptor systems

Morandin, Riccardo 15:00

TU Berlin

Port-Hamiltonian descriptor systems (pHDAE) combine port-Hamiltonian (pH) systems with differential-algebraic equations (DAE), using the language of control systems. PH systems generalize classical Hamiltonian systems to allow dissipation of energy and interaction with the environment, and present inherent passivity and stability properties. The input and output variables are interpreted as "ports" and used for interconnection with other pH systems or with the environment, using energy as a "lingua franca" between different physical domains. The DAE structure allows to include explicitly algebraic constraints into the equations for added robustness, and it is naturally produced by automatic modeling and interconnection.
In this talk we present a general definition for port-Hamiltonian descriptor systems that can deal with finite-dimensional, infinite-dimensional and hybrid systems in the same way, making full use of its flexible differential-algebraic structure to e.g. include boundary control explicitly in the equations, allowing nonlinearities, and permitting even more extensions. The main idea leading to this construction consists in defining skew-symmetric, symmetric and positive (semi)definite operators with respect to certain bilinear forms, which typically combine the inner product of some Hilbert space with boundary contributions. To validate our framework, we present a structure-preserving space-discretization approach based on Galerkin projection, with extensions to time-discretization and model order reduction schemes.

Input-to-state stability for unnbounded bilinear feedback systems

Hosfeld, René (1); Jacob, Birgit (2); Schwenninger, Felix (3); Tucsnak, Marius (4)

1: TU Berlin
2: University of Wuppertal
3: University of Twente, The Netherlands
4: Institut de Mathématiques de Bordeaux

15:20

Input-to-state stability (ISS) is a unifying concept that allows to simultaneously study internal stability and robustness to external controls/perturbations of systems with inputs. Natural sufficient conditions are provided for ISS estimates with respect to small initial conditions and input functions for abstract systems with a linear input and a bilinear feedback term. Both the control and the bilinear feedback, which depend on the state trajectory itself and the output of the system, enter the system through possibly unbounded operators. Moreover, the observation operator associated with the output is also considered to be unbounded.

We apply the obtained results to controlled versions of a viscous Burger equation, a Schrödinger equation, a Navier-Stokes equation and a semilinear wave equation.

S24: History of applied mathematics and mechanics

Organizer(s): Altenbach, Holm *(Otto-von-Guericke-Universität Magdeburg)*

S24.01: History of applied mathematics and mechanics

Date: March 19, 2024 16:30–18:30
Room: G22/112
Chair(s): Altenbach, Holm
Bruhns, Otto Timme

Some remarks on Lode angle and Lode parameter

Bruhns, Otto Timme 16:30
Ruhr University Bochum

In the literature on plasticity, the variables Lode angle and Lode parameter are increasingly used as coordinates to describe the stress space when defining suitable yield or limit conditions - often, however, without any or only alleged reference to the original work of W. Lode. The present considerations will try to close this obvious gap.

Karl Schellbach (1804–1892) – one of the fathers of the Finite Element Method?

Ullrich, Peter 16:50
University of Koblenz

Calculations by aerospace and automotive engineers in the 1950s for industrial applications are usually viewed as the beginnings of the Finite Element Method (FEM). However, some of its basic ideas can already be found on earlier occasions. One of the examples already discussed in the literature, e.g. [Stein 2018, pp. 154–155], is the treatment of the brachistochrone problem by Gottfried Wilhelm Leibniz (1646–1716) in [Leibniz 1697], even if he did not rigorously prove his ideas there.

The mathematics educator Karl Schellbach (1804–1892) appears to have provided the first proof for the brachistochrone problem using FEM-like methods in his article [Schellbach 1851]. (For Schellbach's vita, see e.g. [Ullrich 2019].) However, one has to look at the details: Schellbach certainly first solves some elementary problems of the calculus of variations by discretizing the situation [Schellbach 1851, §§ 2–9]. But then he generalizes this method in order to derive the general Euler-Lagrange equation [Schellbach 1851, §§ 10]. And only on the basis of this differential equation and by use of standard methods from differential calculus he deals with the problem of the brachistochrone [Schellbach 1851, §§ 13–14].

In the final sections of his article, Schellbach generalizes his method to higher dimensions, which makes his considerations appear even more FEM-like. For example, in his treatment of Plateau's problem he begins by dividing the domain of definition into triangles [Schellbach 1851, § 30], which is even shown in an illustration.

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• Ullrich, Peter: Karl Schellbach (1804-1892), Mathematiker des Monats 2019, Berliner Mathematische Gesellschaft, https://www.math.berlin/mathematiker/karl-schellbach.html

„The fruit trees were in full bloom and the weather allowed coffee to be taken outdoors." New Perspectives on the History of the Association of Applied Mathematics and Mechanics (GAMM) 1920-1970

Lemberg, Jason 17:30
University of Wuppertal

When Friedrich Adolf Willers (1883-1959), the long-standing editor of the Journal of Applied Mathematics and Mechanics (ZAMM), enjoyed the spring weather in Darmstadt in 1950, he also expressed his satisfaction of what appeared to be the first meeting of a unified GAMM after a devastating war. The society had been founded in 1922 to represent the interests of applied mathematics and mechanics and as a forum for exchange and it had managed to position itself as a science policy player both during the Weimar Republic and the Third Reich. After the Second World War, however, its continued existence seemed to be in serious jeopardy and the 1950 expression of Willers of the "GAMM in its old form" proved to be deceptive.

The precarious unity of a society that was now spread across four occupation zones and found its counterpart in the open question of the political constitution of Germany serves as the starting point for a new examination of the history of a society in three political systems. For this purpose, new, previously unused source material from several archives will be analyzed. This will be done in two steps: First, a general outline of the history of the society since its beginnings will provide information, locate central actors in their historical context and ask for their science political interests and possibilities. This will be followed by an in-depth look at thematic examples. Particular attention will be paid to the international orientation of the society.

This is a new research project, which is currently set up and which is supported by GAMM.

On the Heritage of Kurt Magnus in Gyro Technology

Wagner, Jörg Friedrich 17:50
University of Stuttgart

Kurt Magnus (1912-2003) is undoubtedly one of the personalities who shaped research and teaching in mechanics during the 20th century. Through his work with his teacher and doctoral supervisor Max Schuler at the University of Göttingen, gyro technology became his most important field of work, which also led to his research in oscillations and later in multi-body systems and mechatronics. K. Magnus made significant international scientific contributions in all these fields. He was regarded as a gifted lecturer, and the close connection between research and practical application was important to him.

His seven-year deportation to the USSR in 1946 was, however, also of central importance in K. Magnus' life. During this time, he was able nevertheless to continue his scientific work under certain restrictions. After his return to Germany, he became Professor of Mechanics at the University of Stuttgart in 1958. His appointment coincided with the gradual resumption of industrial activities in Germany in the field of gyro technology - activities that had come to a standstill at the end of World War II. In the years that followed, K. Magnus' institute became the scientific center for gyro technology in Germany. The activities of that time are reflected in a preserved collection of gyro instruments for research and teaching as well as in the co-founding of an annual international conference for inertial systems, which still exists today. K. Magnus' subsequent move to the Technical University of Munich in 1966 did nothing to change this. At the time, K. Magnus was regarded as a doyen of gyro technology.

After a short biography of K. Magnus, the contribution deals with two topics that have emerged from his work in the field of gyro technology. The first is the recent revision and digitization of the aforementioned gyro collection using photogrammetry and computed tomography as part of the BMBF-funded

project Gyrolog. The second topic is the development of the aforementioned symposium, which provides information on how gyro and inertial technology has developed since the work of K. Magnus in Stuttgart.

Timoshenko and the Creation of new Elements in Teaching Mechanics

Altenbach, Holm
Otto von Guericke University Magdeburg

18:10

Stepan Prokopovich Timoshenko/Stephen P. Timoshenko (December 22 [old style December 10] 1878 in Shpotovka, Chernigov Governorate, Russian Empire – May 29, 1972 in Wuppertal, Germany) was an ethnic Ukrainian, citizen of the Russian Empire and later, an American engineer and academician. He made fundamental contributions to mechanics, among them the now so-called Timoshenko-Ehrenfest beam theory. At the same time, he significantly reformed the engineering education in Russia and the U.S.A., linking elements of academic knowledge with practical problems and emphasizing the specifics of experimental investigations. The starting point of this development was his visit to Göttingen/German Empire. The lecture pay attention to some the new elements in the teaching mechanics.

S25: Computational and mathematical methods in data science

Organizer(s): Pfeffer, Max *(University of Göttingen)*
Nestler, Franziska *(TU Chemnitz)*

S25.01: Various topics in Computational and mathematical methods in data science

Date: March 19, 2024 08:30–10:30
Room: G22/H2
Chair(s): Pfeffer, Max

On the approximation of vector-valued functions by samples

Kressner, Daniel (1); Ni, Tingting (1); Uschmajew, André (2)
1: EPFL, Switzerland
2: University of Augsburg
08:30

The approximation of a vector-valued function by a k-dimensional subspace plays an important role in dimension reduction techniques, such as reduced basis methods. Considering functions f in L^2 Lebesgue-Bochner spaces, the smallest attainable error of such an approximation is characterized by the singular values of f. However, for practical reasons, the linear subspace is often restricted to be spanned by samples of f. By extending a well-known result by Deshpande et al. on column subset selection for matrices, we show that there always exist k samples of f such that the resulting subspace approximation is quasi-optimal with a mild constant.

Learning stochastic reduced order models from data

Freitag, Melina A. (1); Nicolaus, Jan Martin (1); Redmann, Martin (2)
1: University of Potsdam
2: Martin Luther University Halle-Wittenberg
08:50

This work introduces a non-intrusive model order reduction method by extending the operator inference approach to linear and controlled stochastic differential equations with additive noise. The reduced drift and diffusion coefficients are inferred. To this end, appropriate least-squares problems are constructed aiming to fit observational data. Additionally, different subspace constructions based on the available data are compared. A theoretical analysis shows the closeness of the reduced order model (ROM) obtained by the proposed method to the intrusive ROM obtained by POD. Numerical results are presented, depicting the error in expectation and covariance, as well as the weak error, of both ROMs.

A time-aware tensor decomposition for concept evolution

Chatzis, Christos (1,2); Schenker, Carla (1); Pfeffer, Max (3); Lind, Pedro (2); Acar, Evrim (1)
1: Simula Metropolitan Center for Digital Engineering AS, Norway
2: Oslo Metropolitan University
3: University of Göttingen
09:10

Time-evolving data are frequently represented as higher-order tensors with one of the modes being the time mode. For instance, neuroimaging signals might be arranged as a tensor of subjects-by-voxels-by-time, while social network data could be structured as a users-by-words-by-time tensor.

Tensor factorizations have emerged as effective unsupervised methods for analyzing such higher-order datasets and extracting the underlying patterns. However, they frequently overlook the temporal dimension. For instance, a reordering of the time points is allowed, which, although technically permissible, could result in a dataset that describes a fundamentally different evolution of events. Yet, these methods lack the capability to recognize or reflect these significant alterations in the data's temporal structure.

In recent studies, temporal regularizers are incorporated into the time mode to tackle this issue. Nevertheless, existing approaches still do not allow underlying patterns to change in time (e.g., spatial changes in the brain, contextual changes in topics). In this talk, we introduce the temporal PARAFAC2

(tPARAFAC2) model, a PARAFAC2-based tensor factorization with temporal regularization to compute a time-aware factorization of the input with the goal of extracting gradually evolving patterns, which is essential for understanding the data's continuous development through the underlying temporal dynamics. We use an Alternating Optimization (AO) - Alternating Direction Method of Multipliers (ADMM) based algorithm to fit the model and study different algorithmic approaches to handle missing data when fitting the model.

Using numerical experiments on simulated and real data, we demonstrate the effectiveness of tPARAFAC2 model in terms of recovering the underlying (evolving) patterns accurately in various challenging cases, in particular, in the presence of missing entries.

A novel univariate feature selection filter-measure based on the reduction of class overlapping

Liaw, Jin Cheng; Geu Flores, Francisco 09:30
University of Duisburg-Essen

Classification algorithms applied on high-dimensional and imbalanced datasets suffer from high computational cost and performance degradation. While several studies have emphasized the obstacle that class imbalances present, Prati et al. [1] has shown that not only class imbalances are to blame but also the degree of overlapping among the classes. In this contribution, we propose PDE-Segregate, a univariate filter-based feature selection (FS) method based on a filter-measure that ranks features according to their ability to segregate the probability density estimates (PDE) of each unique class.

PDE-Segregate's filter-measure is computed by first normalizing every feature vector such that it ranges from 0 to 1. The samples are then grouped into their respective classes and used to construct PDEs for each class using a kernel density estimator with Gaussian kernels and Scott's Rule for bandwidth selection [2]. Finally, the filter-measure of each feature is computed by numerical integration as the intersection of the areas below all the PDE-curves for the given feature. Features with a low filter-measure value (lower degree of class overlapping) are preferred over those with a higher filter-measure value.

To investigate the performance of our method, we carried out classification experiments on six real microarray benchmark datasets by combining the proposed method with standard classifiers, such as support vector machine, k-nearest neighbor, linear discriminant analysis and naive Bayes. PDE-Segregate performed as well as state-of-the-art FS methods such as Relief-F and MultiSURF [3] and, in some cases, better. One major advantage of PDE-Segregate is that it allows for a visualization of each selected feature's ability to distinguish between classes, which could be helpful for inductive research. Two major limitations of PDE-Segregate include only handling numerical features and requiring enough samples for constructing robust PDEs.

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On Efficient and Accurate Kernel-Based Interpolation/Regression for Dynamic Datasets

Kapadia, Harshit; Feng, Lihong; Benner, Peter 09:50
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Kernel-based techniques like the radial basis function interpolation and Gaussian process regression are widely employed to perform interpolation/regression tasks. For these techniques, one typically resorts to deciding the values of kernel parameters via hyperparameter tuning, e.g., cross-validation and maximum likelihood estimation. However, in scenarios where the dataset under consideration

changes dynamically, it becomes necessary to re-apply the hyperparameter selection strategies, resulting in increased computational costs. Moreover, equipping a uniform width for all the kernels and fixing their positions limits the expressive power of the interpolant/regressor considerably. Our work intends to alleviate this situation by proposing a comprehensive strategy for learning the center location for each kernel, along with center-dependent locally-adaptive kernel widths. More specifically, we present an alternating dual-staged iterative training (ADSIT) procedure that efficiently learns the output layer weights and the kernel parameters associated with the activation functions in a kernel-based shallow neural network (KSNN).

By testing on arbitrary functions, we illustrate an improved performance of the KSNN, trained via the ADSIT procedure, for various interpolation and regression tasks. Furthermore, we showcase the applicability of the proposed ideas in carrying out interpolation/regression for high-dimensional data collected from partial differential equations, specifically in the context of surrogate modeling and data-driven model order reduction for parametric dynamical systems.

S25.02: Various topics in Computational and mathematical methods in data science

Date: March 19, 2024 16:30–18:30
Room: G22/H2
Chair(s): Nestler, Franziska

Neural ODE for Hamiltonian Systems with Irregular and Noisy Data

Janik, Konrad; Goyal, Pawan; Benner, Peter
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg
16:30

Learning generalizing models from measurements is a challenging task, especially when the data is noisy or irregular. Real data is almost never noise-free and often irregular. Therefore noise removal is necessary if we want to learn good models.
In this work we will focus on Hamiltonian systems, which can fully be described by the associated Hamiltonian. We discuss a methodology for learning the Hamiltonian from noisy measurements. To do this we train a neural network to implicitly represent the data.We simultaneously use a Hamiltonian-Neural-Network (HNN) to learn the Hamiltonian and combine both networks by the neural ODE approach.
Another important property of Hamiltonian systems is their symplectic phase flow. If we want to predict future states of the system, we can learn an explicit symplectic integrator by using intrinsic structure-preserving symplectic networks (SympNets). We also combine the SympNets with the implicit representation of the data via the neural ODE approach to deal with noise or irregular measurements. The proposed method can handle data where dependent variables are not available on the same time grid. This is particularly remarkable since standard SympNets only work on equidistant full state variables.
We show the effectiveness of the proposed method by comparing it against standard HNNs and SympNets which do not consider noisy or irregular data.

Functional SDE approximation inspired by a deep operator network architecture

Eigel, Martin; Miranda, Charles
Weierstrass Institute for Applied Analysis and Stochastics
16:50

Stochastic differential equations (SDEs) have emerged as a crucial framework for modelling systems affected by random factors, thereby introducing a stochastic element into solutions. They find extensive use in finance, optimal control, generative models and physical systems. Recently, polynomial chaos expansions have proved to be highly successful in the area of uncertainty quantification of parametric partial differential equations. To date, the potential of polynomial chaos expansion has not been fully exploited for SDE. The main disadvantage in the truncated polynomial chaos expansion is that the number of components grows drastically with the maximum degree of polynomial chaos and the number of basis elements. This talk introduces a new model class, SDEONet, which is founded on the Wiener chaos expansion structure and the concept of Deep Operator Networks. This model

aims to tackle the issue of exponential complexity by learning a sparse truncation of the Wiener chaos expansion. Experiments have validated the suggested approach in 1D and higher dimensions, and we obtain encouraging results.

Approximating Langevin Monte Carlo with ResNet-like Neural Network Architectures
Eigel, Martin; Miranda, Charles; Schütte, Janina Enrica; Sommer, David
Weierstrass Institute for Applied Analysis and Stochastics
17:10

We sample from a given target distribution by constructing a neural network which maps samples from a simple reference, e.g. the standard normal distribution, to samples from the target. To that end, we propose using a neural network architecture inspired by the Langevin Monte Carlo (LMC) algorithm. Based on LMC perturbation results, we show approximation rates of the proposed architecture for smooth, log-concave target distributions measured in the Wasserstein-2 distance. The analysis heavily relies on the notion of sub-Gaussianity of the intermediate measures of the perturbed LMC process. In particular, we derive bounds on the growth of the intermediate variance proxies under different assumptions on the perturbations. Moreover, we propose an architecture similar to deep residual neural networks and derive expressivity results for approximating the sample to target distribution map.

Blending Finite Volume Fluxes with Reinforcement Learning
Schmickler, Sophia Ruth; Gassner, Gregor
University of Cologne
17:30

There is a growing interest in enhancing or substituting traditional numerical methods with machine learning approaches. This presentation specifically targets the improvement of numerical methods. We investigate the feasibility of training an agent to find a high accurate and stable numerical scheme. The target application is solving PDEs using the finite volume method, where the critical decision involves selecting a numerical flux. We employ a convex combination of the Local Lax Friedrich Flux and the central flux. The former, being highly dissipative, is considered low order, while the latter, although second order on an equidistant grid, tends to introduce unphysical oscillations. The task now is to find a good combination of the two fluxes.

To address this challenge, we implement a Reinforcement Learning approach to train an agent tasked with determining the optimal convex combination. The goal is to achieve a stable and highly accurate simulation. In Reinforcement Learning an agent interacts with an environment and tries to optimise its behaviour based on received rewards. We will present how to design the environment and establish a reward structure. Initially, we validate this concept by applying it to the Burgers Equation, subsequently extending our evaluation to the one-dimensional shallow water equations.

Extending denoising diffusion generative models by respecting physical constraints
Bastek, Jan-Hendrik (1); Sun, Steve WaiChing (2); Kochmann, Dennis M. (1)
1: ETH Zurich
2: Columbia University, USA
17:50

Generative models, particularly denoising diffusion models [1], have shown remarkable success in learning complex, high-dimensional probability distributions. Their application has extended beyond creating lifelike images and videos, playing an important role in scientific machine learning, e.g., to address inverse design problems, such as the design of metamaterials with complex (e.g., nonlinear) target properties. [2]

In latter settings, the required training data is typically generated from forward simulators such as the finite-element method, which is then used to train the model based on a data-driven objective. Notably, this leaves the model unaware of the actual physical laws governing the data generation, as typically described by a system of partial differential equations.

We present a novel method to embed these physical principles within the probabilistic framework of denoising diffusion models and improve the model's understanding of generating realistic samples

– not only requiring it to follow the implied training data distribution but also respecting the underlying physics. Furthermore, we extend the formulation to also include inequality constraints and optimization objectives, and present various numerical studies highlighting the potential of using this additional knowledge to train such model classes.

References:

[1] Ho, J., Jain, A., Abbeel, P. (2020). Denoising Diffusion Probabilistic Models. *arXiv:2006.11239*

[2] Bastek, J.-H., Kochmann, D. Inverse-design of nonlinear mechanical metamaterials via video denoising diffusion models. *Nature Machine Intelligence*, to appear

S25.03: Various topics in Computational and mathematical methods in data science

Date: March 20, 2024 08:30–09:30
Room: G22/H2
Chair(s): Neumayer, Sebastian

Greedy Sampling for Parameter Estimation in Partial Differential Equations

Forootani, Ali; Chellappa, Sridhar; Kapadia, Harshit; Goyal, Pawan; Benner, Peter 08:30
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Partial differential equation parameter estimation is a mathematical and computational process used to estimate the unknown parameters in a partial differential equation model from observational data. This paper employs a greedy sampling approach based on the Discrete Empirical Interpolation Method to identify the most informative samples in a dataset associated with a partial differential equation to estimate its parameters. Greedy samples are used to train a physics informed neural network architecture which maps the nonlinear relation between spatio-temporal data and the measured values. To prove the impact of greedy samples on the training of the physics informed neural network for parameter estimation of partial differential equation, their performance is compared with random samples taken from the given dataset. Our simulation results show that for all considered partial differential equations, greedy samples outperform random samples, i.e. we can estimate parameters with a significantly lower number of samples while simultaneously reducing the relative estimation error. A Python package is also prepared to support different phases of the proposed algorithm, including data prepossessing, greedy sampling, neural network training, and comparison.

Structure preserving inference of mechanical systems

Filanova, Yevgeniya (1,2); Pontes Duff, Igor (2); Goyal, Pawan (2); Benner, Peter (2,1) 08:50
1: Otto von Guericke University Magdeburg
2: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Constructing mechanical models based on experimental or simulation data becomes more and more relevant in engineering practice. On the one hand, the mechanical models, identified from experimental measurements, can be used for analysis and simulation. On the other hand, the models used in modern simulation software often need further reduction and should be re-constructed from the simulation results, because the original system operators are very difficult or impossible to access. Moreover, the identified mechanical system should be able to represent the system behavior for a longer time period and different load cases, which means that the original system properties and structural characteristics should be preserved. Due to the specific second-order ODE structure of the governing system of equations, in many cases not all of the system matrices can be reconstructed. In our work, we propose a methodology for the identification and reduction of mechanical systems from data via solving an optimization problem using some ideas from machine learning. We are able to identify all the system operators and preserve their original mathematical properties by including a reasonable parametrization of the system operators in the optimization problem. For linear mechanical systems, this ensures stability and interpretability of the resulting surrogate model. Additionally, we study systems with nonlinear material behavior and the possibility of applying non-intrusive reduction methods to them. Numerical experiments are performed using simulation data from finite element software.

Learning Linear and Quadratic Dynamical Systems with Guaranteed Stability
Pontes Duff, Igor; Goyal, Pawan; Benner, Peter 09:10
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Learning dynamical systems is an emerging field that combines data-driven modeling tools with physics-based modeling, optimization, and empirical knowledge. It plays an essential role in engineering design cycles and digital twinning. In this talk, we primarily focus on an operator inference methodology that builds preferably low-dimensional dynamical models, with a prior hypothesis on the model structure, often determined by known physics or given by experts. Then, for inference, we aim to learn the operators of a model by setting up an appropriate optimization problem. One of the critical properties of dynamical systems is stability. However, stability is not guaranteed by the inferred models. In this work, we propose inference formulations to learn linear and quadratic models, which are stable by design. Precisely, we first study the case of linear dynamical systems and investigate how to impose Lyapunov stability using a matrix parametrization. Then, based on these results, we discuss the parameterization of quadratic dynamical systems that are locally and globally stable. Moreover, for quadratic systems with no stable point yet bounded (e.g., chaotic Lorenz model), we discuss how to parameterize such bounded behaviors in the learning process. Using those parameterizations, we set up inference problems, which are then solved using a gradient-based optimization method. We present several numerical examples, illustrating the preservation of stability and discussing its comparison with the existing state-of-the-art approach to infer operators.

S25.04: Various topics in Computational and mathematical methods in data science

Date: March 20, 2024 14:00–16:00
Room: G22/H2
Chair(s): Uschmajew, André

A Recursive Multilevel Algorithm for Deep Learning
Jacob, Isabel; Ulbrich, Stefan 14:00
TU Darmstadt

As the use cases for neural networks become increasingly complex, modern neural networks must also become deeper and more intricate to keep up, indicating the need for more efficient learning algorithms. Multilevel methods, traditionally used to solve differential equations using a hierarchy of discretizations, offer the potential to reduce computational effort.
In this talk, we combine both concepts and introduce a multilevel stochastic gradient descent algorithm that accelerates learning through a multilevel strategy. A gradient correction term is needed to establish first-order consistency. We discuss additional conditions including step size regularization and an angle condition that ensure the convergence of the method.
To demonstrate the usefulness of our approach, we apply it to residual neural networks in image classification. The resolution of the images is utilized to generate data sets of varying complexity, which are then used to build a hierarchy of neural networks with a decreasing number of variables. Additionally, we construct corresponding prolongation and restriction operators. Numerical results are presented.

Frank-Wolfe Algorithms for Abs-smooth functions
Tadinada, Sri Harshitha (1); Pokutta, Sebastian (2); Walther, Andrea (1) 14:20
1: Humboldt-Universität zu Berlin
2: Zuse Institute Berlin

Many applications involve the minimization of a real valued function f subject to a compact and convex constraint set C. In particular, it is interesting to solve this minimization problem for an abs-smooth f. In a nutshell, the class of abs-smooth functions captures all non-smooth functions whose non-differentiability arises as a result of the absolute value function (eg. max, min, squared loss of a neural network possessing the ReLU or hinge loss activation). A way to solve such minimization problems is via the Abs-Smooth Frank-Wolfe (ASFW) algorithms. The main idea of this method is to first

approximate our original function f with its piece-wise linearization fpl, and then to perform the conditional gradient method (Frank-Wolfe algorithm) on this linearization fpl to reach our minima. The key here is to have a good enough approximation fpl of f, and AD tools like ADOL-C can help us in constructing a good approximation.

Conditional gradient descent methods have regained their popularity in the last few decades, due to the fact that very less computational effort is required in solving a linear minimization oracle (LMO) in each iterative step. Needless to say these algorithms have seen many applications in various fields of optimization and data science. The ASFW algorithms have now been made available as a Julia package. Similar to the smooth Frank-Wolfe algorithms, there are also different variants of the ASFW algorithm - Vanilla ASFW, Lazified ASFW and Stochastic ASFW to name a few. The user has the choice to choose one of these variants depending on the complexity of the given problem and the availability of the given data. These ASFW algorithms have been observed to give similar expected results as of the smooth Frank-Wolfe algorithms, which have been studied extensively. With the availability of these ASFW algorithms, we can now tackle a class of non-smooth optimization problems (optimization of abs-smooth functions).

Iteratively Reweighted Least Squares Recovery on Tensor Networks

Kraemer, Sebastian 14:40
RWTH Aachen University

One fundamental approach to matrix recovery, being a predecessor to tensor recovery, traces back to the affine rank minimization problem. While there are various surrogate approaches within that setting, we emphasize here that the asymptotic minimization of the well-known, so called *log-det* objective functions always yields the desired, minimal rank matrices within the given, affine set; whereas such may or may not recover an a-priorly sought for ground truth. Concerning the commonly applied method of iteratively reweighted least squares (IRLS-0), one thus remains with two concerns. How problematic are local minima inherent to the log-det approach truly; and opposingly, how influential instead is the numerical realization. With higher dimensions in mind, based on the concept of matricization, affine sum-of-ranks minimization then generalizes the setting from matrices to tensors. While convergence properties are directly transferable, we demonstrate that in numerical experiments, the corresponding IRLS-0 method can be exhausted in order to observe the theoretical phase transition for generic tensor recoverability. In large-scale applications in turn, alternating, reweighted optimization on tensor tree networks allows to avoid exponential computational complexity, without substantial loss of approximation quality.

Variationally correct methods for model reduction of parameterized transport equations by neural networks

Bachmayr, Markus; Dahmen, Wolfgang; Oster, Mathias 15:00
RWTH Aachen University

Linear transport equations with parameterized vector fields and non-smooth data are an interesting class of models for which classical model order reduction methods based on linear subspace approximation are inefficient due to slowly decaying Kolmogorov n-widths. This leads us to consider methods beyond linear subspaces. As the solutions to parameterized transport equations exhibit some compositional sparsity, it turns out that the parameter-to-solution map can be well-approximated by deep neural networks such that explicit bounds on the number of neurons and layers can be provided that defy the Curse of Dimensionality for large parameter dimensions. In principle a neural network approximation to the parameter-to-solution map can be trained by minimizing the empirical mean squared error of the prediction to high fidelity snapshots in a desired model-compliant norm. However, generating sufficiently many such snapshots is computationally expensive. Instead we prefer methods that minimize residuals averaged over the parameter set and thus avoid the need of computing solution snapshots. In view of the notorious uncertainty of optimization success with neural networks we insist though on the residual loss quantity to be at every stage of the training process uniformly proportional to the error in a relevant norm. This can be achieved by employing variationally

stable formulations of the PDE. This, however, comes in our case at the price of frequently evaluating a dual norm. To render this task feasible, we use discontinuous Petrov-Galerkin (dPG) techniques since they allow to compute the dual norm of the residual explicitly, once uniform dPG stability has been established. Specifically, we propose a hybrid method that uses a dPG finite element discretization in space and specifically tailored neural networks in the parametric variables. That is, the network takes the parameter vector as input and outputs the coefficients of the spatial basis functions. The network is trained by minimizing the empirical mean of the explicit dPG residuals by means of gradient based schemes. We illustrate the method by judiciously chosen numerical examples which, in particular, shed light on transport-specific obstructions.

On automated model discovery and a universal material subroutine

Linka, Kevin (1); Peirlinck, Mathias (2); Holthusen, Hagen (3); Hurtado, Juan A. (4); Kuhl, Ellen (5) 15:20

1: Hamburg University of Technology
2: TU Delft
3: RWTH Aachen University
4: Dassault Systemes, USA
5: Stanford University, USA

Constitutive modeling is the cornerstone of computational and structural mechanics. In a finite element analysis, the constitutive model is encoded in the material subroutine, a function that maps local strains onto stresses. This function is called within every finite element, at each integration point, within every time step, at each Newton iteration. Today's finite element packages offer large libraries of material models to choose from. However, the scientific criteria for appropriate model selection remain highly subjective and prone to user bias. Here we explore whether and how we can eliminate user involvement and automate material modeling in finite element analysis. We leverage recent developments in constitutive neural networks, machine learning, and artificial intelligence [1] to discover the best constitutive model from thousands of possible combinations of a few functional building blocks [2]. We seamlessly integrate all discoverable models into the finite element workflow by creating a universal material subroutine that contains more than 60,000 models, made up of 16 individual terms [3]. Our results suggest that constitutive neural networks can robustly discover various flavors of arterial models from data, feed these models directly into a finite element simulation, and predict stress and strain profiles that compare favorably with traditional constitutive models. Replacing dozens of individual material subroutines by a single universal material subroutine that is populated directly via automated model discovery–entirely without human interaction–makes finite element analyses more accessible, more robust, and less vulnerable to human error. This could forever change how we simulate materials and structures.

[1] Linka K, Kuhl E. A new family of Constitutive Artificial Neural Networks towards automated model discovery. Comp Meth Appl Mech Eng. 2023; 403:115731.

[2] Linka K, St Pierre SR, Kuhl E. Automated model discovery for human brain using Constitutive Artificial Neural Networks. Acta Biomat. 2023; 160: 134-151.

[3] Peirlinck M, Linka K, Hurtado JA, Kuhl E. On automated model discovery and a universal material subroutine for hyperelastic materials. Comp Meth Appl Mech Eng. 2024; 418: 116534.

Our source code, data, and examples are available at https://github.com/LivingMatterLab/CANN.

S25.05: Various topics in Computational and mathematical methods in data science

Date: March 20, 2024 16:30–18:30
Room: G22/H2
Chair(s): Pfeffer, Max

Sparsity-Inspired Regularization for Image Reconstruction
Neumayer, Sebastian
TU Chemnitz
16:30

In this talk, I will introduce a generic framework for learning filter-based regularization functionals from image data. If we pursue a variational reconstruction ansatz for solving inverse problems, these can be deployed to a variety of different imaging modalities (universality). Further, this ansatz ensures data consistency and we are able to derive some stability guarantees. Obeying with such paradigms is very important when working in critical applications such as medical imaging, since false diagnosis can have fatal consequences. After introducing the baseline architecture, I will discuss an improvement of this architecture via conditioning on the data. In the last part of the talk, I will present numerical results for denoising and MRI. These indicate that even relatively restricted architectures can be able to achieve highly competitive performance.

Analyzing Concrete Pavement Damage Progression Using Image Dataset Techniques
Garita-Duran, Hellen; Kaliske, Michael
TU Dresden
17:10

In the field of pavement damage analysis, long-term damage monitoring and assessment remain a formidable challenge due to the dynamic nature of damage development and environmental changes. This study introduces an approach for tracking and analyzing the progression of pavement deterioration over time using image datasets of real concrete pavement. The research focuses on specific road sections, with annual data collection over five years. This yields a time series dataset with detailed spatiotemporal information. To standardize the dataset, image rectification, and joining processes are applied. This preprocessing ensures that each image is comparable in detail and orientation. The proposed methodology involves integrating GPS data for precise location mapping and employing advanced image analysis techniques to identify and monitor pavement damages consistently across different time frames. This includes analysis of visual characteristics of the damage to ensure consistent tracking. This approach ensures a comprehensive understanding of the damage evolution. A success rate will be obtained that will be critical in illustrating pavement deterioration and assessing the impact of maintenance operations. This approach is relevant to the future of road infrastructure maintenance and rehabilitation strategies as it facilitates timely interventions throughout the pavement life cycle.

Neural Galerkin schemes that can preserve Hamiltonians and other quantities
Schwerdtner, Paul (1); Schulze, Philipp (2); Peherstorfer, Benjamin (1); Berman, Jules (1)
1: New York University, USA
2: TU Berlin
17:30

Neural Galerkin schemes, based on the Dirac-Frenkel variational principle, train nonlinear parametrizations sequentially in time to approximate solution fields of time-dependent partial differential equations. Due to the nonlinearity of the parametrizations, few parameters efficiently capture even complex dynamics in first-principles-based physical models. Such models are often constructed based on the observation that quantities like energy, mass, and momentum remain constant over time, representing conserved quantities of the physical system. In this talk, we demonstrate how we can modify Neural Galerkin schemes such that these quantities are also conserved quantities in the approximate solutions produced by Neural Galerkin schemes. We first show that only adding constraints that aim to conserve quantities in continuous time can be insufficient because the nonlinear dependence on the parameters implies that even quantities that are linear in the solution fields become nonlinear in the parameters and are thus not conserved by standard Runge-Kutta time integration schemes. Instead, we propose Neural Galerkin schemes that compute an embedding onto the manifold of nonlinearly parametrized solution fields that conserve given quantities at each time step. We present numerical experiments that show the effectiveness of our proposed method to preserve given quantities up to machine precision.

Deep Learning for Structure-Preserving Universal Stable Koopman-Inspired Embeddings for Nonlinear Canonical Hamiltonian Dynamics

Goyal, Pawan; Yıldız, Süleyman; Benner, Peter 17:50
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Hamiltonian systems possess several crucial properties, such as a symplectic flow and energy preservation. The preservation of these properties in numerical models can lead to more accurate and stable simulations. In this talk, we present data-driven modeling for nonlinear Hamiltonian systems. This approach enables the construction of simpler models, thereby facilitating prediction, control, and optimization for complex nonlinear Hamiltonian systems. In line with our objective, Koopman operator theory provides a framework for the global linearization of nonlinear systems, which allows for the use of linear tools in design studies. In this work, our focus is on identifying global linearized embeddings for canonical nonlinear Hamiltonian systems through a symplectic transformation. While this task can be challenging, we utilize the strength of deep learning to uncover the desired embeddings. To address the constraints of Koopman operators in systems with continuous spectra, we implement the lifting principle and acquire global cubic embeddings. Furthermore, we emphasize the importance of ensuring stability in the dynamics of the discovered embeddings. We showcase the potential of deep learning in obtaining compact symplectic coordinate transformations and their corresponding simplistic dynamical models. This promotes data-driven learning of nonlinear canonical Hamiltonian systems, even those possessing continuous spectra.

S25.06: Various topics in Computational and mathematical methods in data science

Date: March 21, 2024 08:30–10:30
Room: G22/H2
Chair(s): Stoll, Martin

GAN Enables Outlier Detection and Property Monitoring for Additive Manufacturing of Complex Structures

Henkes, Alexander (1,2); Herrmann, Leon (3); Wessels, Henning (2); Kollmannsberger, Stefan (3) 08:30
1: ETH Zurich
2: TU Braunschweig
3: Technical University of Munich

Additive manufacturing technologies have seen significant economic growth over the past years. Although additive manufacturing processes have matured in many areas, difficulties with regard to printing accuracy persist. Possible defects are, e.g., the generation of unwanted internal pores or a lack of fusion between layers, to name only a few. In general, defects result in a deviation between as-planned and as-built geometries, all of which can be difficult to detect in an automatized fashion. Previous work has shown that image-based simulation can assist in quality monitoring of produced parts and may complement experimental testing. Yet, both experimental testing and simulation-based approaches are involved and not yet directly applicable to all manufactured parts in a series production. The paper at hand suggests a remedy to this problem by using a generative adversarial network (GAN). Generative adversarial networks have shown to be able to emulate as-built geometries of engineering relevance. Moreover, they can realistically reproduce the distributions of such deviations. To this end, we present how this feature can be harvested to employ generative adversarial networks for outlier detection. To this end, we use the discriminator of a GAN as a classifier on as-built parts to judge whether an as-built structure is acceptable or defective. The viability of the approach is demonstrated on basic artificial structures with spherical voids as well as additively manufactured lattice structures whose geometry is acquired after production via computed tomography (CT). The methodology is not only applicable for automated property monitoring but potentially also for reliability estimates of neural network-based property predictors.

Interconnection of port-Hamiltonian systems with port-Hamiltonian Neural Networks

Peters, Till 08:50
TU Braunschweig

Increasingly large and complex dynamical systems play a major role in mathematical modeling today. These complex systems are often disassembled into many small subsystems interacting with each other. In mechanics, electrical circuits or flow dynamics we can often represent these systems and the subsystems as port-Hamiltonian systems. The port-Hamiltonian formulation is a very general structure which is on the one hand based on a Hamiltonian function associated with the total stored energy. On the other hand ports are essential which are interconnected by power-preserving interconnections. Furthermore, the formulation allows us to include dissipation, interconnection and control terms into the possibly implicit differential equations of the system. In [1], Neary and Topcu introduce port-Hamiltonian neural networks (pHNNs) to learn port-Hamiltonian subsystems from data. These pHNNs are port-Hamiltonian systems with trainable neural networks as system matrices. Hence, the port-Hamiltonian properties of the systems are also guaranteed for the pHNNs. Moreover, Neary and Topcu use physics informed interfaces between these submodels to capture their interactions.

Like in [1], we test the coupled spring mass damper example where a chain of masses is interconnected by springs to study the interconnection of port-Hamiltonian systems. We learn the dynamics of the small submodels from training data and then use the trained models with different interconnections to construct a larger model of interconnected subsystems. The accuracy of the constructed model is investigated and also for interconnections that are not known in advance and require little additional data for the large interconnected system. Several types of interconnections of these small port-Hamiltonian systems, e.g. feedback interconnection, yield a larger system with port-Hamiltonian structure again. We compare different interconnections in terms of trajectory approximation and testing loss on additional data.

References

[1] C. Neary and U. Topcu. Compositional Learning of Dynamical System Models Using Port-Hamiltonian Neural Networks. Proceedings of The 5th Annual Learning for Dynamics and Control Conference, Proceedings of Machine Learning Research 211: 679-691, 2023

On minimizing the training set fill distance in machine learning regression

Climaco, Paolo (1); Garcke, Jochen (1,2) 09:10
1: University of Bonn
2: Fraunhofer SCAI

For regression tasks one often leverages large datasets for training predictive machine learning models. However, using large datasets may not be feasible due to computational limitations or high data labelling costs. Therefore, suitably selecting small training sets from large pools of unlabelled data points is essential to maximize model performance while maintaining efficiency. In this talk, we study Farthest Point Sampling (FPS), a data selection approach that aims to minimize the fill distance of the selected set. We derive an upper bound for the maximum expected prediction error, conditional to the location of the unlabelled data points, that linearly depends on the training set fill distance. For empirical validation, we illustrate experiments using two regression models on three datasets. We empirically show that selecting a training set by aiming to minimize the fill distance, thereby minimizing our derived bound, significantly reduces the maximum prediction error of various regression models, outperforming alternative sampling approaches by a large margin. Furthermore, we show that selecting training sets with the FPS can also increase model stability for the specific case of Gaussian kernel regression approaches. Finally, we propose and analyse a variation of FPS considering weighted distances that take into account the distribution of the data during the sampling process. This approach aims to improve the performance of a model by reducing its average prediction error on the data distribution.

Driving on a racetrack with a hybrid reinforcement learning approach
Gottschalk, Simon 09:30
University of the Bundeswehr Munich

In this talk, we focus on a scenario, where a racing car drives over a track and overtakes opponent cars. The special challenge in this task lies in finding a fast controller, which is able to control the car online, and the collision avoidance of cars, which are not only modelled as point masses.

Therefore, we introduce a hybrid method. This method consists of two parts: first, a reinforcement learning (RL) part, which decides on the sequence of target positions to steer to. Secondly, a physics informed surrogate model for the actual control of the vehicle going from the current position to the chosen next one. The idea behind this method is to separate the collision avoidance from finding actual controls for the dynamical system. While the collision avoidance is handled by the RL part, which decide on the position along the route, the actual controls need to be found by solving an optimal control problem. Thereby, finding its solution should not take too much time, since such a problem needs to be solved several times during the controlling phase as well as during the training of the RL agent. Thus, we train a neural network offline based on the Karush-Kuhn-Tucker equations of this problem, which maps the parameters of the problem (like starting and target points) to the solution of the optimal control problem motivated by [1].

Overall, we obtain a controller, which determines the next point along the track first and outputs the actual controls in order to get to this point afterwards. Furthermore, the overall computation is very fast, since we mainly only execute two mappings (e.g. neural networks). In our application case, we see how this controller is able to overtake moving opponents on the racing track and successfully fulfills the task.

[1] A. DeMarchi, A. Dreves, M. Gerdts, S. Gottschalk, S. Rogovs. A Function Approximation Approach for Parametric Optimization. Journal of Optimization Theory and Applications 196, pages 56-77, 2022.

S25.07: Various topics in Computational and mathematical methods in data science

Date: March 21, 2024 14:00–16:00
Room: G22/H2
Chair(s): Nestler, Franziska

Preconditioning the Kernel ANOVA SVM
Stoll, Martin 14:00
TU Chemnitz

We will illustrate how an interior point scheme can be used to solve the SVM quadratic optimization problem. We show that this requires the solution of a large-scale linear system that needs a suitable preconditioner. In many cases it will be necessary to find a fast matrix vector multiplication to deal with the large and dense kernel matrix. For this we suggest the use of a feature grouping approach with an NFFT based ANOVA scheme to improve accuracy and convergence speed. We illustrate the performance on several data sets.

Transformers and Function Approximation: What Can We Learn About the Attention Scheme?
Thesing, Laura 14:20
LMU München

Natural language processing made an impressive jump with the introduction of Transformers. ChatGPT is one of the most famous examples. It is now widely used in society and even forces teachers and professors to rethink the evaluation process of homework assignments. With the performance, it is also changing the perception of the possibilities of AI, even outside the research community. In addition, Transformers are not only a powerful tool for natural language processing but also for other applications, like computer vision and biology.

The main building block of Transformers is the attention scheme. The attention mechanism allows us to connect every element in a sequence with every other element. Therefore, it is substantially different from feedforward networks. However, it also leads to a quadratic cost in the sequence length. For long text, this complexity can be a bottleneck. Therefore, more efficient versions were introduced, which allowed to reduce the time complexity to be linear with a similar performance on benchmark tasks.

Besides the great success of Transformers, there are still a lot of open questions from the theoretical perspective. We approach the investigation of Transformers from two perspectives: we analyse the expressive power of Transformers and efficient Transformers. Moreover, we investigate in experiments how the approximation with Transformers differs from classical approximation schemes and deep feedforward networks.

On the invariance of Gaussian RKHS's under Koopman operators

Philipp, Friedrich (1); Schaller, Manuel (1); Worthmann, Karl (1); Peitz, Sebastian (2); Nüske, Feliks (3)

1: TU Ilmenau
2: Paderborn University
3: Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

14:40

The Koopman operator for stochastic differential equations (SDEs) is a linear operator which provides full information on the expected stochastic dynamics. It is therefore a popular object in the prediction and control of dynamical systems. The Koopman operator is typically unknown, and many data-driven approaches towards its approximation by finite-rank operators have been proposed and analyzed. The most popular of them being Extended Dynamic Mode Decomposition (EDMD). A special kind of EDMD is kernel EDMD (kEDMD), where the dictionary of observables consists of the canonical kernel features evaluated at the data points. In this talk, we present the first bounds on the prediction error of the EDMD and kEDMD estimators. Concerning kEDMD, the result can be extended to the full approximation error if the RKHS is invariant under the Koopman operator. We show that this invariance holds in arbitrary dimensions for Gaussian RKHSs and SDEs with constant coefficients and a dissipative drift matrix. This is a key step towards the characterization of the interplay of SDEs and kernels w.r.t. this often imposed invariance assumption.

Utilizing Machine Learning for Hydrogel Swelling Prediction

Wang, Yawen; Ehrenhofer, Adrian; Wallmersperger, Thomas

TU Dresden

15:00

Hydrogels enable promising applications in sensors and actuators. They can perform unique chemical, optical and mechanical transitions, i.e., swelling or deswelling, in response to external stimuli. Our current research focuses on the swelling behavior of hydrogels, which is one of the most important properties of hydrogels when they are applied as part of sensors or actuators.

Data-driven methods have been widely used in deciphering the Processing-Structure-Properties-Performance (PSPP) relationship of materials in the field of materials informatics. It inspires us to apply artificial neural networks (ANNs) in predicting the swelling behavior of hydrogels based on their processing procedure. In the current research, we introduce a very specific approach: predicting discrete swelling states of temperature-responsive hydrogels based on their synthesis parameters, utilizing ANN models.

We analyze the literature on temperature-responsive hydrogels, from which we summarize essential synthesis parameters and extract the relevant data points accordingly to build the database. We propose three variants of ANN models. After comparing their performance in the acquired database, the one presenting the best accuracy in predicting the swelling states within the test dataset is selected. This approach can be applied to previously predict the expected properties based on the "material fingerprint" of hydrogels, before they are synthesized and validated experimentally.
The current model can still be improved in two ways: First, we can enrich the database by applying automated tools, e.g., Large Language Models, in extracting data points from literature; or collecting

experimental data through the cooperation with chemists in the lab. Second, we can use machine learning techniques to get a better model with limited data. A potential technique can be transfer learning. A pre-trained model trained by the big source data can then be tuned with the limited data of hydrogels. We can analyze the pre-trained models from the existing model libraries of other passive and active materials, and evaluate if they are suitable to be adapted in predicting the properties of hydrogels.

S26: Modeling, analysis and simulation of molecular systems

Organizer(s): Matera, Sebastian *(Fritz Haber Institute of the MPS)*
Herbst, Michael *(Ecole Polytechnique Federale de Lausanne (EPFL))*

S26.01: Embedding and correlated methods

Date: March 19, 2024 08:30–10:30
Room: G22/209
Chair(s): Stamm, Benjamin
Friesecke, Gero

Mathematical insights on embedding theories.

Kirsch, Alfred (1,2)
1: CERMICS, École Nationale des Ponts et Chaussées
2: Matherials, INRIA

08:30

In the field of electronic structure calculation,*embedding theories* are algorithms designed to access many-body electronic properties through a *self-consistent two-level scheme computation*, itselfbased on a so-called *fragmentation* of the one-particle space. The *high-level* solver gives an *accurate* computation for each of the *small* and *interacting fragments,* while the *low-level* solver returns an *average* but*global* quantity.

Depending on the set of observables to compute and the application field, several algorithms have been designed : in the condensed matter community, the Dynamical Mean-Field Theory (DMFT) [1] has been thoroughly used for almost three decades to study strongly interacting systems by computing the one-particle Green's functions, while in the chemistry community, Density Matrix Embedding Theory (DMET) [2] continues to be increasingly used to approximate the one-particle reduced density matrix of molecules of larger and larger size.

In spite of their great use, very few mathematical studies [3,4,5] have been carried out to understand the properties of these algorithms : in this talk, I will introduce some of them and present results on their well-posedness and exactness [6]. If time allows, I will conclude on numerical examples.

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5. M. Lindsey, "The Quantum Many-Body Problem: Methods and Analysis." Chapter VII, PhD dissertation, 2019.

6. Cancès, Éric, Fabian M. Faulstich, Alfred Kirsch, Eloise Letournel and Antoine Levitt. “Some mathematical insights on Density Matrix Embedding Theory.” arxiv:2305.16472, 2023.

Multi-center decomposition of molecular densities: A numerical perspective

Cheng, YingXing 08:50
University of Stuttgart

Atom-in-molecule (AIM) analysis, critical in computational chemistry, involves partitioning molecular density into atomic contributions using weight functions, thereby defining atoms within molecules. Optimization is achieved using functions like the Kullback-Leibler entropy.
Various methods like QTAIM, Iterative Stockholder Analysis (ISA), and Hirshfeld have been developed, with ISA being more effective but computationally intensive compared to Hirshfeld.
Previous research [J. Chem. Phys. 156, 164107 (2022)] evaluated alternative, cost-effective AIM methods and introduced a unified framework based on Kullback-Leibler entropy, encompassing the ISA, ISA with Gaussian basis functions (GISA), Hirshfeld, Iterative Hirshfeld (Hirshfeld-I), Additive Variational Hirshfeld (AVH), and Minimal-Basis ISA (MB-ISA) methods.
This framework introduces naturally a new linear approximation of ISA method, L-ISA, suitable for mathematical analysis, including existence, uniqueness of the composition, and its convergence.

In this talk we will give an update on recent developments on the fast and accurate implementation of the iterative solver in order to solve the non-linear equations determining the solution.

Parallel Coordinate Descent Methods for Full Configuration Interaction

Zhang, Yuejia; Gao, Weiguo; Li, Yingzhou 09:10
Fudan University, China

Solving the time-independent Schrödinger equation gives us full access to the chemical properties of molecules. Among all the ab-initio methods, full configuration interaction (FCI) provides the numerically exact solution under a predefined basis set. However, the FCI problem scales exponentially with respect to the number of bases and electrons and suffers from the curse of dimensionality. The FCI problem could be reformulated as an unconstrained minimization problem. This work proposes a novel algorithm to address the minimization problem. The algorithm introduces an extra search dimension to enable the exact line search for the multi-coordinate descent method, which could be fully parallelized. Hence, the proposed algorithm benefits from both exact line search and parallelization. Numerically, we demonstrate the parallel efficiency of the algorithm. The algorithm achieves better energy and parallelism on systems with approximately a hundred electrons than other existing methods.

On algebraic varieties and roots in coupled cluster theory

Faulstich, Fabian Maximilian (1); Sturmfels, Bernd (2); Sverrisdóttir, Svala (3) 09:30
1: Rensselaer Polytechnic Institute, USA
2: Max Planck Institute for Mathematics in the Sciences, Leipzig
3: University of California, Berkeley, USA

We develop algebraic geometry for the coupled cluster (CC) theory of quantum many-body systems. The high-dimensional eigenvalue problems that encode the electronic Schrödinger equation are approximated by a hierarchy of polynomial systems at various levels of truncation. The exponential parametrization of the eigenstates gives rise to truncation varieties. These generalize Grassmannians in their Plücker embedding. We provide a detailed study of truncation varieties and their CC degrees, and we present the state of the art in solving for all roots to the CC equations.

Coupled Cluster for Periodic Systems

Schneider, Reinhold 09:50
TU Berlin

We consider the Coupled Cluster method applied to periodic systems, e.g bulk crystal.

The periodic structure is handeld by the Bloh Floquet transformation with a large super-cell convergni got the thermo-dynamic limit. Although the Coupeld Cluster approximation is established as a highly accurate wave approximation in qunatum chemistry application, its application for periodic systems is limited due to its unfavourable complexity. We show that the amplitudes depend on the k indices on the dual lattice admits a certain regularity, whoch allow compressibility by wavelet representation, althogh admits a certain low rank factorization ot QTT(quantized tensor trains) representaton.

S26.02: Solvation models and Molecular Dynamis

Date: March 19, 2024 16:30–18:30
Room: G22/209
Chair(s): Nüske, Feliks
Matera, Sebastian

Exploring Electrostatic Effects in Aqueous Nanosystems: From Continuum Models to Classical Force Field Simulations and Machine Learning

Loche, Philip 16:30
EPFL, Switzerland

Electrostatic phenomena, like lightning in a thunderstorm or a balloon sticking to our hair, are ubiquitous in our day-to-day life. These phenomena are based on the forces exerted by electric charges, as described by Coulomb's law. Although initially developed for macroscopic objects, Coulomb's law holds with astonishing accuracy on the nanoscale, describing interactions among atoms, molecules, and ions—the building blocks of all matter. A molecule of utmost importance in natural science is water. An exact electrostatic description of liquid water and its interaction with other dissolved molecules or ions is challenging due to the complex structure of the liquid. Therefore, we often resort to a continuum description, treating water as an unstructured, homogeneous dielectric material. This approach explains several phenomena, such as ion solvation or colloid precipitation. However, it is known that at interfaces, the isotropy and homogeneity of water's dielectric properties break down. Indeed, any modification of the dielectric constant at interfaces or in confined spaces fundamentally influences all electrostatic interactions, including the equilibria of chemical reactions or particle distributions.

The dielectric properties of water and ions can be well quantified using classical force field atomistic simulations. In these simulations, long-range interactions, such as electrostatics or dispersion, are very well described. Thus, we can use classical force field simulations to analyze the dielectric properties of matter. We will provide an overview of extracting these properties from atomistic simulations, how electrostatic interactions are modified in aqueous nanosystems, and how well a dielectric continuum description performs compared to recent experiments.

However, classical simulations have limitations as they do not account for the quantum nature of the chemical bond, which usually manifests itself on short time and length scales. Electronic structure calculations offer an accurate description of both quantum and long-range effects but are computationally demanding and scale poorly with system size. Therefore, over the last decade, machine learning (ML) approaches have emerged as an effective strategy to build surrogate models that provide comparable accuracy at a fraction of the computational cost. A crucial ingredient in many ML-based methods for atomistic modeling of materials and molecules is the use of locality. While this allows for better system-size scaling, it systematically neglects long-range (LR) effects such as electrostatic or dispersion interactions. In addition to the analysis of classical simulations of aqueous nanosystems, we also present an extension of the long-distance equivariant (LODE) framework. This framework can handle diverse long-range interactions in a consistent manner and integrates seamlessly with preexisting ML methods. The method allows for a direct physical interpretation of these interactions via the multipole expansion, facilitating simpler and more efficient implementations. This allows us to study atomistic system that have significant long-range effects at the same accuracy as electronic structure calculations.

A L^2 maximum principle on the disk with applications to continuum solvation models

Carvalho Corso, Thiago (1); Stamm, Benjamin (1); Jha, Abhinav (1); Hassan, Muhammad (2) 17:10
1: University of Stuttgart
2: EPFL, Switzerland

In this talk we discuss a new convergence-analysis of the Schwarz domain decomposition method for solving Laplace's equation in the union of two or more disks in 2D. The critical step relies on a novel L^2 version of the maximum principle for interior arcs on the disk, whose proof relies on a detailed analysis of the Poisson kernel on the strip in the complex plane. As an application, we can derive explicit (and in some cases optimal) geometry-dependent rates of convergence for algorithms used in implicit solvation models such as the (ddCOSMO) algorithm introduced by Cances, Maday, and Stamm in 2013.

Julia MolSim: Bridging the Gap between Mathematical Research and Practical Applications in Molecular Simulations

Travelletti, Cédric; Herbst, Michael 17:30
EPFL, Switzerland

Mathematical research in atomistic modelling of molecules and solids suffers from difficulties in transfering new ideas to actual production codes. Indeed, there is currently a gap between the molecular simulation frameworks that researchers use to develop new algorithms and the ones that are used in practice. This gap makes it difficult to test new ideas on real applications and to scale them to production environment, thus limiting the amount of feedback that math researchers can get from the user side. In this presentation, we introduce the Julia MolSim ecosystem, that aims at building a bridge between research and application communities by providing a fully integrated environment for atomistic simulations. By centralizing different aspects of atomistic modelling, Julia MolSim allows mathematicians to test new algorithms against multiple backends while also streamlining application to real-world problems. It provides functionalities for visualizations, IO and HPC workflow management that help researcher transition from the prototyping phase to actual testing on real applications. We will demonstrate those capabilities by focusing on the problem of geometry optimization, showcasing how Julia MolSim allows new algorithm ideas to be prototyped and tested in the same framework. Furthermore, by leveraging the integration of Julia MolSim with the AiiDA infrastructure, we display how new geometry optimization algorithms can be quickly brought to bear on problems in large-scale computational materials discovery. To summarize, our goal is to show how the use of composable software can be a game changer in the development of new mathematics for molecular simulations by bridging the gap between researchers and end users.

Complex Activation and Catalytic Cycles of Deubiquitinylase Enzymes

Ilter, Metehan; Stein, Matthias 17:50
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

Ubiquitination is a marker signal for a controlled protein degradation. Deubiqutinylases are enzymatically removing these ubiquitin markers from proteins and controlling many protein signalling pathways. Bacteria and viruses possess also deubiquitinating enyzmes which allow to circumvent to host's innate immune system.

Molecular Dynamics simulations covering several microseconds are needed in order to shed light on the activation mechanisms of members of the OTU subfamily of deubiquitinylases. This process requires the use of all-atom simulations and the defintion of structural parameters that are able to describe the state of activation of the OTU protein. The process of activation and catalytic turnover of the OTU Cezanne-1 is a multistage cycle with several critical dynamic transitions that cannot be characterized based on static protein structures alone.

Sufficient sampling of the complex structural dynamics is required in order to fully exploit the conformational transitions along the catalytic cycle. Probability densities are converted to free energy contour maps and allow the assignment of different energy minima in various states of the protein.

For example, the ubiquitin-free Cezanne-1 dynamically shuttles between catalytically competent and incompetent states which suggests that its activation is independent of substrate binding. The catalytically competent substrate-free Cezanne-1 promotes distal ubiquitin substrate access to the catalytic center. Subsequent binding of the proximal ubiquitin shifts the equilibrium toward the catalytically competent state of the dyad, thereby promoting proteolysis of the iso-peptide bond. After cleavage of the scissile bond, sequential dissociation of first the proximal ubiquitin induces the inactivation of Cezanne-1. The subsequent release of the distal ubiquitin fully reconstitutes the inactive substrate-free state of Cezanne-1.

Molecular dynamics-based investigation of polymer fracture
Ries, Maximilian; Weber, Felix; Steinmann, Paul; Pfaller, Sebastian
FAU Erlangen-Nürnberg
18:10

Polymers and polymer composites offer high stiffness and strength at comparably low densities and are thus vital for lightweight designs, e.g., in automotive and aerospace applications. However, the fracture behavior of polymers has yet to be fully understood from an engineering point of view since the crack propagation is governed by molecular effects such as bond scission, chain sliding, formation of cavities, and crazing. Therefore, we present a molecular dynamics (MD) based investigation of the fracture behavior of amorphous thermoplastics. To this end, we employ an extended Kremer-Grest bead-spring model, which captures the generic material behavior of polymers. We subject the samples to novel non-periodic boundary conditions to mimic a double-cantilever test, well known in macroscopic fracture mechanics. In contrast to conventional periodic MD simulations, this setup permits us to make initial conclusions about crack propagation and, thus, fracture toughness in amorphous polymers. This first contribution will pave the way for more elaborate FE-MD multiscale approaches to unravel the fracture behavior of polymers and polymer composites.

S26.03: Various topics

Date: March 20, 2024 08:30–09:30
Room: G22/209
Chair(s): Matera, Sebastian
Friesecke, Gero

Energy-Driven Decision-Making Across Biological Systems: From Gene Regulation to Population Dynamics
Kumar, Rajneesh; Johnston, Iain George
University of Bergen, Norway
08:30

Decision-making in individual cells, and cellular populations, is a fundamental aspect of biological systems, influencing processes ranging from developmental biology to ecological responses. While recent experimental work has revealed substantial cell-to-cell differences in energy availability (ATP), the influence of energy supply on this cellular decision-making remains theoretically underexplored. We aim to explore the common thread of energy dependency in decision-making across different biological scales, delving into fine-grained modeling approaches to understand the intricate relationship between ATP availability and decision-making capacity.

At the single-cell level, we explore the emergence of cell fate attractors in a range of toggle switch models as ATP levels vary, demonstrating that higher energy levels support increased decision-making capacity. We use both deterministic and stochastic modeling of individual molecular players (in contrast to previous coarse-grained approaches) to explore the influence of ATP on the noisy dynamics of cell decision-making. Further, we bridge the scale to decision-making in cellular populations to explore how organisms adapt their behavior in response to environmental changes. Here, we model organisms with two primary behaviors: a resting state and active environmental exploitation, and the (energetically costly) ability to switch between them in response to environmental change. Our findings highlight the importance of environmental energy availability, with the understanding that sensing the environment incurs an energy cost. In dynamic environments, informed decision-making

proves advantageous, provided the energetic cost is manageable. Conversely, in stable environments with high energetic costs, uncontrolled strategies emerge as more favorable.

This unified investigation emphasizes the overarching significance of energy dynamics in decision-making processes, connecting molecular events in gene regulation to macroscopic behaviors in population dynamics. By investigating these phenomena across different biological scales, we contribute to a more comprehensive understanding of how energy availability influences the adaptive strategies of biological systems. This integrated perspective facilitates multidisciplinary research by, bridging the gap between molecular and ecological studies in the context of energy-driven decision-making.

Shape-driven simulation of protein self-assembly

Mayrhofer, Lukas (1); Evans, Myfanwy (2); Friesecke, Gero (1)
1: Technical University of Munich
2: University of Potsdam

08:50

Protein self-assembly is a large-scale process that cannot be replicated using all-atom molecular dynamics simulations. We develop a coarse-grained model with the goal of simulating this process for the tobacco mosaic virus, where the coat proteins self-assemble into a helical shell.

We base our approach on the premise that the geometric shape of the protein drives the solvation. The shapes interact via a standard volume term promoting overlap and an interpenetration penalty. To efficiently realize the Gibbs measure on the space of possible configurations we employ the hybrid Monte Carlo algorithm together with a careful use of signed distance functions for energy evaluation.

Numerical experiments in 2D reveal certain essential features for robust self-assembly, including non-convexity of the shape and nonuniformity of the interaction along the boundary (i.e. local attraction and repulsion). Initial simulation results in 3D for the coat protein of the tobacco mosaic virus are also shown.

We showcase an interactive simulation tool that we developed in Julia to enable efficient identification of suitable simulation parameters.

Uncertainty quantification for molecular statics via implicit differentiation

Maliyov, Ivan (1,2,3); Grigorev, Petr (1,2,3); Swinburne, Thomas D (1,2,3)
1: Aix-Marseille University, France
2: CNRS, France
3: Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), France

09:10

Molecular statics simulations depend sensitively on the parameters of any interatomic potential. Gauging the effect of parameter uncertainty on results typically requires expensive resampling. In this work, we developed an implicit derivative technique to evaluate the energy of relaxed minima to the second order in parameter variation. While automatic differentiation routines have powerful generality and are efficient, they incur large memory requirements, saturating best-in-class GPU memory even for thousands of atoms. Instead, we have designed a sparse linear operator technique for highly parallel and memory-efficient computations. The method is implemented as an efficient constrained minimization routine, compatible with any molecular dynamics package. The approach has been implemented in the LAMMPS and JAX-MD packages and applied to the calculation of defect formation energies and stability of dislocation cores, demonstrating its ability to solve a wide range of uncertainty propagation and inverse design tasks in atomistic simulation.

S26.04: Tensor methods and DMRG

Date: March 20, 2024 14:00–16:00
Room: G22/209
Chair(s): Schneider, Reinhold
Herbst, Michael

Tensor-Based Approaches for Modeling and Simulation of Molecular Systems

Gelß, Patrick 14:00
Zuse Institute Berlin

In this presentation, we delve into tensor-based methodologies applicable to diverse scientific domains. Drawing from recent publications, our exploration spans chemical dynamics, machine learning, and quantum mechanics, employing innovative techniques to unravel the complexities of molecular interactions. Beginning with a comprehensive overview of tensor decompositions, with a primary focus on the tensor-train (TT) format, we shift our attention to the realm of chemical reaction networks and associated master equations. Leveraging TT-based solvers for linear equations and eigenvalue problems, we showcase the computation of stationary distributions. Expanding our analysis to metastable sets within molecular dynamics, we afterwards explore transfer operators and demonstrate the capabilities of low-rank data representations. The presentation then briefly addresses tensor-based algorithms for broader machine learning tasks, such as the multidimensional approximation of nonlinear dynamical systems and neural-network training. Concluding with a glance into quantum-mechanical systems, including coupled exciton-phonon systems and quantum circuits, we underline the versatility and efficacy of tensor-based approaches. These diverse contributions collectively demonstrate the power and applicability of tensor-based approaches in advancing the understanding and simulation of molecular systems, offering new perspectives for researchers at the intersection of physics, chemistry, and computational science.

Symmetries and tensor train representation of electronic wave functions

Badreddine, Siwar (1); Cancès, Eric (2); Dupuy, Mi-Song (3); Grigori, Laura (4) 14:40
1: INRIA, France
2: ENPC, France
3: Sorbonne Université
4: EPFL, Switzerland

DMRG (Density Matrix Renormalisation Group) has become a state-of-the-art method to solve the many-body body electronic eigenvalue problem. It relies on a parametrisation of the wave function in the Fock space as a tensor train (also called matrix product state).

The electronic wave function satisfies several symmetries such as the particle number, the azimutal spin and the total spin symmetries. The first two are abelian symmetries which induce a block sparse representation of the cores of the tensor train (TT) representation of the wave function. The total spin symmetry is a SU(2) symmetry, which implies a more intricate form of the TT representation of the wave function. In this talk, symmetry-preserving TT representations will be presented.

Numerical Experiment on changing tensor network topology in DMRG calculations for strongly correlated systems.

Boamah, Elizabeth Adomako 15:00
Technical University of Munich

The study of strongly correlated systems via the Density Matrix Renormalization Group (DMRG) method has predominantly been constrained to specific network topologies, mainly linear chains and periodic structures. However, the intricate nature of quantum entanglement in these systems suggests that exploring a wider array of tensor network topologies could yield significant insights. This research initiates an extensive comparative study of DMRG performance across various network topologies, beginning with linear and periodic configurations, and extending to more complex structures in future investigations.

Our initial focus is on analyzing how DMRG performs in traditional linear chain topologies versus periodic (ring-like) systems, specifically observing changes in energy and other quantum properties during the transition from linear to periodic topology. This foundational comparison sets the stage for a broader exploration of how different network configurations can impact the efficacy of DMRG calculations.

Looking ahead, the study aims to incorporate a range of innovative and unconventional topologies. The objective is to understand how modifications in the network structure influence the accuracy, computational efficiency, and the ability of DMRG to capture the complex quantum states inherent in strongly correlated materials.

This ongoing research is expected to provide a comprehensive understanding of the relationship between tensor network topology and DMRG performance. The findings will not only contribute to the optimization of DMRG methods for existing models but also pave the way for new approaches in studying quantum many-body systems. The implications of this work are far-reaching, potentially influencing future developments in quantum computing, material science, and beyond.

Predicting the Full CI energy of large systems to chemical accuracy from restricted active space density matrix renormalization group calculations

Friesecke, Gero (1); Barcza, Gergely (2); Legeza, Ors (2,3)

1: Technical University of Munich
2: Wigner Research Centre for Physics, Budapest, Hungary
3: Institute for Advanced Study, Technical University of Munich

15:20

We theoretically derive and validate with large scale simulations a remarkably accurate power law scaling of errors for the restricted active space density matrix renormalization group (DMRG-RAS) method in electronic structure calculations. This yields a new extrapolation method, DMRG-RAS-X, which reaches chemical accuracy for strongly correlated systems such as the Chromium dimer, dicarbon up to a large cc-pVQZ basis, and even a large chemical complex like the FeMoco with significantly lower computational demands than previous methods. The method is free of empirical parameters, performed robustly and reliably in all examples we tested, and has the potential to become a vital alternative method for electronic structure calculations in quantum chemistry, and more generally for the computation of strong correlations in nuclear and condensed matter physics.

Reference: https://arxiv.org/abs/2209.14190, to appear in Journal of Chemical Theory and Computation

S26.05: Eigenvalue problems and Gross-Pitaevskii equation

Date: March 20, 2024 16:30–18:30
Room: G22/209
Chair(s): Matera, Sebastian
Nüske, Feliks

Error scaling of the restricted active space density matrix renormalization group method.

Máté, Mihály (1,2); Friesecke, Gero (1); Legeza, Örs (2,1)

1: Technical University of Munich
2: Wigner Research Centre for Physics, Budapest, Hungary

16:30

The restricted active space density matrix renormalization group (DMRG-RAS) method, a recently introduced technique for calculating ground state energies with chemical accuracy in strongly correlated systems, is investigated thoroughly in this study. The focus includes an analysis of the error bounds of the method, exploring the trade-off between the size of the active space and configurations within the restricted active space, as well as the scalability towards higher excitation levels. Recognizing the basis dependence of tensor network state methods, including DMRG-RAS, we employ different basis sets in our study, and utilize orbital optimization [2]. The performance of the DMRG-RAS method is compared with other state-of-the-art electronic structure methods, such as coupled cluster approaches.

[1] G. Friesecke, G. Barcza, Ö. Legeza. Predicting the FCI energy of large systems to chemical accuracy from restricted active space density matrix renormalization group calculations. arXiv:2209.14190 [physics.chem-ph]

[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)

Reduced basis surrogates for quantum spin systems based on tensor networks

Brehmer, Paul (1); Herbst, Michael F. (2); Wessel, Stefan (3); Rizzi, Matteo (4,5); Stamm, Benjamin (6)
1: University of Vienna, Austria
2: EPFL, Switzerland
3: RWTH Aachen University
4: University of Cologne
5: Jülich Supercomputing Centre, Forschungszentrum Jülich GmbH
6: University of Stuttgart

16:50

In this talk, we present a reduced basis method for quantum spin problems. Within the reduced basis methods approach, an effective low-dimensional subspace of a quantum many-body Hilbert space is constructed in order to investigate, e.g., the ground-state phase diagram. The basis of this subspace is built from solutions of snapshots, i.e., ground states corresponding to particular and well-chosen parameter values. Here, we show how a greedy strategy to assemble the reduced basis and thus to select the parameter points can be implemented based on matrix-product-states (MPS) calculations using DMRG-optimization. Once the reduced basis has been obtained, observables required for the computation of phase diagrams can be computed with a computational complexity independent of the underlying Hilbert space for any parameter value. We illustrate the efficiency and accuracy of this approach for different one-dimensional quantum spin-1 models.

Numerical simulation of the Gross–Pitaevskii equation via vortex-tracking

Carvalho Corso, Thiago (1); Kemlin, Gaspard (2); Melcher, Christof (1); Stamm, Benjamin (3)
1: University of Stuttgart
2: LAMFA, Université de Picardie Jules Verne, Amiens, France
3: RWTH Aachen University

17:10

This talk deals with the numerical simulation of the Gross–Pitaevskii (GP) equation, for which a well-known feature is the appearance of quantized vortices with size of an order parameter ε. Without a magnetic field and with suitable initial conditions, these vortices interact, in the singular limit ε=0, through an explicit Hamiltonian dynamic. Using this analytical framework, we will present a numerical strategy based on the reduced-order Hamiltonian system to efficiently simulate the infinite-dimensional GP equation for small but finite ε. This method allows us to avoid numerical stability issues in solving the GP equation, where small values of εtypically require very fine meshes and time steps. We will also provide a mathematical justification of our method, in terms of good supercurrent approximation, as well as some numerical experiments.

Using a posteriori error estimators to construct low-cost solution strategies for the Gross-Pitaevskii equation

Hassan, Muhammad (1); Maday, Yvon (2); Wang, Yipeng (2)
1: EPFL, Switzerland
2: Laboratoire Jacques-Louis Lions, Sorbonne Université

17:30

The numerical resolution of a PDE usually requires the introduction of a discretisation space and the use of an iterative solver to approximate the solution of the PDE on this discrete space. A typical approach is to successively enlarge the dimension of the discretisation space while performing solver iterations in each approximation space until a convergence threshold is met. The choice of these successive dimensions and the number of solver iterations for each approximation space together constitute a *solution strategy*, and it is natural to ask how to construct solution strategies of minimal computational cost that achieve a given target accuracy.

In this talk, we discuss the application of a posteriori error estimators for constructing low-cost solution strategies for Gross-Pitaevskii-type equations on the torus. The core idea of our proposal is to minimise the iteration error on coarse discretisations before jumping to a judiciously chosen, much larger approximation space and performing only a few solver iterations. This approach is motivated

by structural insights gleaned from optimal solution strategies for model problems and supported by a super-convergence result for Galerkin solutions of Gross-Pitaevskii-type equations.

S26.06: Transport, dynamics and learning

Date: March 21, 2024 08:30–10:30
Room: G22/209
Chair(s): Herbst, Michael
Stamm, Benjamin

Learning effective dynamics via kernel-based approximation of Koopman generator

Nateghi, Vahid; Nüske, Feliks
Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg

08:30

Accurately detecting the coarse-grained coordinates is an essential task in the model discovery of complex systems, such as molecular dynamics. In many cases, such systems cannot 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 the identification of stochastic dynamical systems. However, the selection of basis functions upon which the generator is approximated is a non-trivial task and needs to be done manually. 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 a dynamical system. This 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 and molecular dynamics problems.

Boltzmann Generators as Optimal Transport Problems

Winters, Quinn Campbell; Friesecke, Gero
Technical University of Munich

08:50

Normalizing flows are a class of neural networks used in machine learning to approximate diffeomorphisms between two spaces and allow for quick sampling from complicated distributions. Recently, normalizing flows have been used by Noe and coauthors to simulate molecular dynamics [1] - first, one trains a neural network that can transform samples from a latent variable, such as a high-dimensional gaussian vector, into a sample from a Boltzmann distribution for the molecular system, and then calculate observables of the system by averaging over many samples generated by the neural network that have been appropriately re-weighted to account for rare events in both the latent variable and the target distribution.

Unfortunately, due to singularities in common energy functionals, such as those used in the Leonard-Jones model, these techniques are not always theoretically justified. In this talk, we present techniques for regularizing the target Boltzmann distribution, and justify the existence of diffeomorphisms for the regularized problems through well known facts in the regularity theory of optimal transport. We will also present numerical simulations to show the efficacy of such techniques in sampling equilibrium states include for many-body problems.

[1] https://doi.org/10.1126/science.aaw1147

Active, Multi-Fidelity Learning for Efficient Molecular Machine Learning

Zaspel, Peter
University of Wuppertal

09:10

In molecular machine learning, we are interested to predict properties of molecules such as ground state energies, excitation energies or dipole moments. These quantities are regularly calculated by approximately solving the Schrödinger equation. Highly accurate approximations are computationally expensive. Therefore, we are interested to replace such calculations on larger classes of molecules or

molecular trajectories by efficient learning models. Still, for high accuracy in the data, the generation of the necessary training data can become very expensive.

In this talk, we discuss ongoing research on the construction of highly accurate machine learning models, where we at the same time keep the total time for generating the training data at a minimum level. In a multi-fidelity approach, we exploit the hierarchy of quantum chemical methods and basis set sizes to reduce cost based on an extension of the so-called Delta-ML approach. In active learning, we greedy-optimally select training samples (instead of using random training samples) to build more versetile predictive models.

This is joint work with Matthias Holzenkamp, Ulrich Kleinekathöfer, Dongyu Lyu, Sayan Maity and Vivin Vinod.

Artificial Intelligence based detection of local spots in network materials prone to mechanical failure.

Bachhav, Bhagyashri; Wu, Zhao; Markert, Bernd; Bamer, Franz 09:30
RWTH Aachen University

Predicting failure in non-crystalline solids like silica glass is challenging due to the complex nature of the fracture process. The failure originates from specific local zones of certain sizes where the atomic structure is highly susceptible to local rearrangement [1]. The Local Yield Stress (LYS) Method predicts such locations of plastic events during external deformation [2]. Despite the precise prediction accuracy of the location of the failure initiation, the mentioned method requires substantial computational resources as it evaluates each local zone separately for rearrangement and is time-consuming. Owing to new age development in artificial neural networks, a relation can be established between the plastic events and the atomic structure. In this study, a neural network is trained to identify this relation and, hence, predict the location of the atomic rearrangement [3]. This approach results in a surprisingly reliable heatmap indicating soft spots that highly correlate with the fracture process and allows for reliable incorporation of structural identification to coarser mechanical frameworks that need local information for a physically meaningful description. The advantage of this method is that it can be trained on a specific atomic structure of a particular material and can predict the local soft spots for unseen structural information without the need for multiple time-consuming molecular simulations.

[1] F. Bamer, F. Ebrahem, B. Markert, B. Stamm, Arch. Comput. Methods Eng. 30 (2023) 2105-2180.
[2] S. Patinet, D. Vandembroucq, M.L. Falk, Phys. Rev. Lett. 117 (2016), 045501.
[3] K. Kontolati et al., Acta Mater. 215 (2021), 117008.

Coupling continuum and high fidelity models with multilevel on-the-fly sparse grids

Hülser, Tobias; Matera, Sebastian 09:50
Fritz-Haber-Institut der Max-Planck-Gesellschaft

Many simulations of continuum models require the repetitive evaluation of some non-linear functions. If these functions are only implicitly given by the outcome of a high-fidelity simulation, these evaluations can easily become the computational bottleneck of the coupled simulation.

To overcome this limitation, computationally efficient machine-learning models have become popular as surrogates of the high-fidelity model in the continuum scale simulation. However, if the input dimension of the high-fidelity model is high, the training of the surrogate often requires infeasible numbers of simulations, the so-called curse of dimensionality.

We present an on-the-fly adaptive sparse grid approach which lifts these limitations. This approach utilizes that sparse grids are comparatively mildly affected by the curse of dimensionality and their hierarchical structure allows for adaptive local grid refinement, i.e. a local approximation error-based training set design. Further, it exploits that during a continuum simulation, only a small low-dimensional subset of the high-dimensional input space of the high-fidelity model is visited. For the employed sparse grid basis, this allows to construct the surrogate on the fly during the continuum simulation and to omit most of the expensive simulations compared to training beforehand - without

affecting the simulation results. The hierarchical structure of sparse grids further allows a straightforward formulation of the coupled problem as a multilevel Newton approach to further reduce the high-fidelity evaluations.

We exemplify the approach on a physical-chemical model from the field of heterogeneous catalysis, where a high-fidelity microkinetic model is coupled to a one-dimensional continuum model for a fixed-bed reactor. We demonstrate the reduction of the number of necessary high-fidelity evaluations for a single coupled simulation but also for parametric scans. We find that, already for the former case, our strategy can save orders of magnitude of high-fidelity evaluations, depending on the targeted accuracy. Additionally, parametric scans profit from the reuse of already conducted high-fidelity results. The savings are particularly pronounced for high numbers of grid points employed for the discretization of the continuum model. Thus, the approach seems to be particularly suited for complex continuum models, e.g. Computational Fluid Dynamics simulations and poses a promising route for coupling these with demanding high-fidelity models, e.g. molecular simulations.

S26.07: Various Topics

Date: March 21, 2024 14:00–16:00
Room: G22/209
Chair(s): Hassan, Muhammad
Schneider, Reinhold

A Quasi Time-Reversible Grassmann extrapolation of density matrices for accelerating Born-Oppenheimer molecular dynamics

Pes, Federica (1); Polack, Étienne (2); Mazzeo, Patrizia (1); Dusson, Geneviève (3); Stamm, Benjamin (4); Lipparini, Filippo (1)
1: University of Pisa
2: École des Ponts ParisTech, France
3: Université de Franche-Comté, France
4: University of Stuttgart

14:00

Born-Oppenheimer molecular dynamics (BOMD) is a powerful but expensive technique. The main bottleneck in a density functional theory (DFT) BOMD calculation is the solution to the DFT nonlinear equations that requires an iterative procedure that starts from a guess for the density matrix. To speed up such calculations, various extrapolation strategies have been developed to use densities available at previous simulation steps as a guess for the iterative procedure. However, density matrices belong in a Grassmann manifold, which is not a vector space. Therefore the linear extrapolation is performed in a tangent space of the manifold, thanks to a locally bijective map between the manifold and its tangent space. In this contribution, we introduce the so-called Quasi Time-Reversible scheme based on Grassmann extrapolation (QTR G-Ext) of density matrices for an accurate calculation of initial guesses. Some numerical experiments show excellent results, namely, the method clearly reduces the number of self-consistent field iterations compared to the state of the art, and at the same time achieves energy-conserving simulations.

A posteriori error analysis of a linear Schrödinger type eigenvalue problem for atomic centered discretizations

Dupuy, Mi-Song (1); Dusson, Geneviève (2); Lygatsika, Ioanna-Maria (1)
1: Sorbonne Université
2: Université de Franche-Comté, France

14:20

In this talk, we present a first *a posteriori* error analysis for variational approximations of the ground state eigenpair of a linear Schrödinger type eigenvalue problem for systems with one electron and M atoms, whose electronic structure is governed by a linear Hamiltonian operator. The variational approximation of the ground state eigenpair is based on a Gaussian discretization of size N centered on atoms. We provide *a posteriori* estimates of the error in the energy norm regarding the Hamiltonian operator, when N goes to infinity. We introduce the residual of the equation and decompose it into M residuals characterizing the error localized on atoms. It is shown that the bound can be expressed

in terms of the dual "local" norms induced by the radially symmetric operators centered on atoms. Such bound is fully computable as soon as an estimate on the dual local norms of the local residuals is available, which is obtained by performing a spectral decomposition of the bounded Hydrogen-like operators. Finally, we provide numerical illustration of the performance of such a posteriori analysis on test cases.

A Posteriori Error Analysis for Kohn-Sham Equations with Convex Exchange-Correlation Functionals

Lainez Reyes, Rafael Antonio 14:40
University of Stuttgart

Ab initio simulations are widely employed in Chemistry, Materials engineering and other fields; a common problem, tackled with Ab initio simulations, is approximating the ground state of an electronic system, and among the most popular models are the Kohn-Sham models. Frequently, the Kohn-Sham equations are numerically solved using an iterative scheme known as Self-Consistent field Iteration. In this talk we will introduce guaranteed error bounds for this numerical scheme for Kohn-Sham Equations with Convex Exchange-Correlation Functionals. We will then show how to decompose this bound into a part depending on the discretization and one depending on the iterative scheme itself. Finally we will present some examples to test the validity of the theoretical results. This is a joint work with Bordignon, A., Cancès E., Dusson, G., Kemlin, G, Stamm, B.

Applying a Well-Defined Energy Density for Machine-Learned Density Functionals

Polak, Elias; Vuckovic, Stefan; Zhao, Heng 15:00
University of Fribourg, Switzerland

The recent integration of machine learning techniques in density functional theory (DFT) has established a powerful framework for developing next generation density functionals. While robust modelling of the exchange-correlation requires a well-defined energy density, conventional training sets usually rely on global quantities. We propose the application of the local slope in the non-interacting limit of the adiabatic connection approach in DFT [1]. The talk will elucidate the methods for an efficient implementation of this quantity, with a focus on its spin-resolved components and its regularized version. Furthermore, we will highlight the potential of this strategy in paving the way for the next generation of machine-learned local dynamic hybrid functionals. Our results show a marked improvement in the prediction of observables while also maintaining computational efficiency.

References

[1] S. Vuckovic, T. J. P. Irons, A. Savin, A. M. Teale, and P. Gori-Giorgi, “Exchange–Correlation Functionals via Local Interpolation along the Adiabatic Connection”, Journal of Chemical Theory and Computation 12, 2598–2610 (2016).

Moreau-Yosida Regularization in Density-Functional Theory

Laestadius, Andre 15:20
Oslo Metropolitan University

The universal density functional is everywhere discontinuous in the standard formulation of density-functional theory. The Moreau-Yosida transformation is a tool from convex analysis that allows us to regularize in a lossless way as far as the energy is concerned. In this talk I will outline the theoretical basis and how this regularization can be used to formulate density-functional theory. Furthermore, the link between Moreau-Yosida regularization and density-potential inversion will be discussed.

Alphabetical Speaker Index