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Contents

1 Plenary Lectures

Ludwig Prandtl Memorial Lecture 06.03.2017 14:00-15:00
Chair: Martin Oberlack (Technische Universität Darmstadt) Weimar hall, Large hall

Some variants of classical multiphase flow problems

Howard Stone (Princeton University)

I will briefly discuss three problems that have classical roots and in each case seek to add one new feature to a modern version of the problem. In the first problem the Saffman-Taylor viscous fingering problem is discussed for the case that there are geometric variations in the flow directions – we show via experiments and theory that such changes can significantly modify the stability features of the flow. In the second problem we consider the low Reynolds number motion of a hot sphere in a fluid accounting for the variations of the viscosity with temperature – we show that the Lorentz Reciprocal Theorem provides a means to construct an analytical representation of the force and torque on the sphere for the case of small viscosity variations. Finally, we present experiments of unexpected dynamics in modest Reynolds number flows at a T-junction and rationalize the results by demonstrating the connections to vortex breakdown.

Plenary Lecture 1 06.03.2017 15:00-16:00
Chair: Jörg Schumacher (TU Ilmenau) Weimar hall, Large hall

The h-principle in fluid mechanics: non-uniqueness and energy dissipation

László Székelyhidi (Leipzig)

It is known since the pioneering work of Scheffer and Shnirelman in the 1990s that weak solutions of the incompressible Euler equations behave very differently from classical solutions, in a way that is very difficult to interpret from a physical point of view. Nevertheless, weak solutions in three space dimensions have been studied in connection with a long-standing conjecture of Lars Onsager from 1949 concerning anomalous dissipation and, more generally, because of their possible relevance to Kolmogorov's K41 theory of turbulence. In joint work with Camillo De Lellis we established a connection between the theory of weak solutions of the Euler equations and the Nash-Kuiper theorem on rough isometric immersions. Through this connection we can interpret the wild behaviour of weak solutions of the Euler equations as an instance of Gromov's celebrated h-principle. In this lecture I will explain this connection and outline the most recent progress concerning Onsager's conjecture.

Plenary Lecture 2 06.03.2017 16:30-17:30
Chair: Carsten Könke (Bauhaus-Universität Weimar) Weimar hall, Large hall

Stochastic structural mechanics - from probability theory to structural design

Christian Bucher (Wien)

Structural mechanics since its beginnings has developed very strongly with respect to more accurate modelling and analysis. A key role in this development play numerical methods, especially those based on the concept of finite elements. This high degree of presision, however, is undermined by imprecise and/or incomplete knowledge about the describing parameters of the models and the environmental actions on the structures, such as e.g. wind or earthquakes. Even with a substantially increased effort for experimental evidence, it is frequently not possible to arrive at deterministic descriptions for these parameters. Therefore uncertainty-based (e.g. probabilistic) analysis becomes mandatory. This lecture will highlight some selected points how stochastic structural mechanics can contribute to solve open problems related to the development of structural design procedures.

Plenary Lecture 3 06.03.2017 17:30-18:30
Chair: Thomas Hotz (TU Ilmenau) Weimar hall, Large hall

Uncertainty Quantification: Propagation and Inference

Oliver Ernst (Chemnitz)

The dynamically growing scientific discipline of Uncertainty Quantification (UQ) addresses the numerous sources of uncertainty in complex simulations of scientific and engineering phenomena in order to assess the validity, reliability and robustness of the results of such simulations. In this regard, it represents a key enabling technology for what is now called Predictive Computational Science.
In this talk we focus on two key UQ components. The first, uncertainty propagation, is concerned with solving a random differential equation, by which is meant a differential equation containing uncertain data modeled by a probability law. We highlight recent developments in collocation methods which address the situation where the uncertain data is parameterized by a countably infinite number of random parameters. In the second part of the talk we present numerical methods for performing Bayesian inference on such random data as a systematic way of merging observational data with a given probabilistic model. The challenge here is to efficiently sample from the posterior distribution in an infinite-dimensional state space with cost that is robust with respect to state space resolution and the variance of the observational noise.

Plenary Lecture 4 07.03.2017 11:30-12:30
Chair: Peter Benner (MPI Magdeburg) Weimar hall, Large hall

Model-Reduction in Micromechanics of Materials

Pierre Suquet (LMA, CNRS, Marseille)

A common practice in structural problems involving heterogeneous materials with well separated scales, is to use homogenized, or effective, constitutive relations. In linear elasticity the structure of the homogenized constitutive relations is strictly preserved in the change of scales. The linear effective properties can be computed once for all by solving a finite number of unit-cell problems. Unfortunately there is no exact scale-decoupling in multiscale nonlinear problems which would allow one to solve only a few unit-cell problems and then use them subsequently at a larger scale. Computational approaches developed to investigate the response of representative volume elements along specific loading paths, do not provide constitutive relations. Most of the huge body of information generated in the course of these costly computations is often lost. Model reduction techniques, such as the Non Uniform Transformation Field Analysis, may be used to exploit the information generated along such computations and, at the same time, to account for the commonly observed patterning of the local plastic strain field. A new version of the model will be proposed in this talk, with the aim of preserving the underlying variational structure of the constitutive relations, while using approximations which are common in nonlinear homogenization.

Plenary Lecture 5 08.03.2017 09:00-10:00
Chair: Achim Ilchmann (TU Ilmenau) Weimar hall, Large hall

On the stabilization of control systems

Jean-Michel Coron (Paris)

A control system is a dynamical system on which one can act by using controls. For these systems a fundamental problem is the stabilization issue: Is it possible to stabilize a given unstable equilibrium by using suitable feedback laws? (Think to the classical experiment of an upturned broomstick on the tip of one's finger.) On this problem, we present some pioneer devices and works (Ctesibius, Watt, Maxwell, Lyapunov...), some more recent results, and an application to the regulation of the rivers La Sambre and La Meuse in Belgium. Highlights are put on time-varying feedback laws, hyperbolic 1-D hyperbolic systems as well as positive or negative effects of the nonlinearities.

Richard von Mises Lecture 1 08.03.2017 10:00-11:00
Weimar hall, Large hall

Experimental and numerical study of heterogeneous material behavior in technological processes at different scales

Benjamin Klusemann (Leuphana Universität Lüneburg)

Modern technological processes demand for high performance materials. For such processes, the relation between microstructure, properties and the macroscopic constitutive response is crucial. To interpret and model heterogeneous metallic materials enabling us to design optimal structural properties it is essential to analyze and understand the interactions of different, even competing mechanisms at different length scales. However, the development of various microstructures depending on the chemical composition, loading path and loading rate, makes it a difficult task to elaborate directly comprehensive constitutive models. In this regard it is important to develop and identify sophisticated models for specific mechanisms at the relevant scales and additionally for scale bridging. However, an extended and valid understanding of the different mechanisms can only be obtained in a multidisciplinary context, where experimental observations and model concepts are linked strongly. In this regard, the talk will address different experimental and numerical investigations of heterogeneous materials at different length scales, focusing in particular on the modeling of microstructures, material instabilities as well as its application in technological production processes.

Richard von Mises Lecture 2 08.03.2017 10:00-11:00
Weimar hall, Large hall

Multiscale Dynamics near Instability

Christian Kuehn (TU München)

Multiscale dynamical systems occur in an extraordinary variety of contexts in the natural sciences and engineering. From the scales of quantum mechanics, chemical reactions, and neurons, up to lasers, fluid dynamics, and celestial mechanics, many applications naturally yield widely differing space and time scales. Frequently, this situation provides a doubled-edged challenge for applied mathematics. On the one hand, having several scales available helps for analytical methods. Reducing phase space, gluing several subsystem results and deriving coarse-grained approximations are frequently possible. These strategies are all helpful for pen-and-paper approaches, which may be impossible for a completely general nonlinear dynamical system. On the other hand, several scales tend to complicate numerical simulation as standardized scientific computing methods may become unstable quickly if systems are stiff, or miss key features on subgrid scales. In this talk I shall outline three deceptively simple situations, where general multiscale aspects, and the role of small parameters in particular, are crucial for theoretical as well as practical results. (I) The first class of problems are fast-slow ordinary differential

equations (ODEs) arising in chemical reactions, where substantially differing reaction rates induce multiple time scales. In this context, the main task is to analyse non-stationary reactions producing oscillations. (II) The second class of problems arises in mathematical biology as well as phase-field models, among many other disciplines. In this context, nonlocal partial differential equations (PDEs) with small nonlocality are of key interest for pattern formation. (III) The last example will be drawn from stochastic differential equations (SDEs) with small noise. In many dynamical systems with noise, one has observed in various sciences, that early-warnings extracted from time series may appear before drastic bifurcation-induced transitions. This observation is the motivation to provide a suitable mathematical analysis. The common theme among our examples is the problem of disentangling multiscale dynamics near an instability. One may simply not neglect small effects once the main driving terms are only marginally stable in a mathematical model. This causes a very challenging multi-parameter problem. In particular, we are actually facing a 'curse-of-instability', which requires higher-dimensional models and accompanying novel mathematical analysis.

Plenary Lecture 6 09.03.2017 09:00-10:00
Chair: Klaus Zimmermann (TU Ilmenau) Weimar hall, Large hall

Experimental substructuring: assembly of measured components for noise and vibration analysis

Daniel Rixen (TU München)

Many components in modern product cannot be modeled easily or properly: they need to be characterized experimentally. In vibration analysis of complex structural and mechatronical systems, it is highly desirable to build models of assemblies where some components are modeled numerically (e.g. by Finite Elements) whereas others are characterized experimentally. Building substructured models from experimental measurements enables engineers to rapidly detect troublesome parts, identify excitation sources and optimize the dynamics of their design. Such strategies form the basis of so-called Transfer Path Analysis techniques (TPA).
Although the mathematical theory of TPA is rather straightforward, its mechanical interpretation is not intuitive and applying simple ideas to real measurements is a real challenge. If you think that measurements are always the reality ... think again: measured dynamic properties of structures (typically Frequency Response Functions) are not only inaccurate, but do often not even satisfy fundamental mechanical properties such as passivity or reciprocity. Such errors render a straightforward application of the theory illusory.
In the presentation, we will discuss a framework to describe the simple algebra needed in substructuring techniques for structural vibration analysis and we will discuss how the vibration source of active components can be indirectly measured. Also we will outline some important tricks and twists that are needed to use measured components in an assembly. The methods will be illustrated on an industrial example.

Plenary Lecture 7 09.03.2017 10:00-11:00
Chair: Tom Lahmer (Bauhaus-Universität Weimar) Weimar hall, Large hall

Beyond uniaxial tension - current trends in experimental mechanics

Stefan Diebels (Saarbrücken)

The phenomenological approach of continuum mechanics is based on axioms and on experiments. While the balance equations are accepted as physical laws experiments form the basis of constitutive modelling, e.g. the quality of a stress-strain relation at finite deformations strongly depends on the underlying data. On the one hand, experiments leading to homogeneous stress and strain states are typically preferred due to their simple evaluation. On the other hand, multiaxial stress and deformation states are required to match the three dimensional state in a real component. Even if it is still an unsolved task to measure inhomogeneous stress distributions in a specimen, optical strain measurement became a very powerful tool to reconstruct the inhomogeneous displacement field at least on the surface of a specimen. Therefore, the evaluation of inhomogeneous experiments, e.g. true biaxial tests, offers new possibilities in the validation of constitutive equations. In most cases, due to the inhomogeneity and the non-linearity of the resulting boundary value problem, the identification of the material parameters becomes an inverse problem. The present contribution addresses the application of modern experimental techniques for the design of experiments, their realisations and, finally, the parameter identification. Special focus is given to inhomogeneous experiments and to the miniaturisation of experiments.

Plenary Lecture 8 09.03.2017 11:30-12:30
Chair: Hans Babovsky (TU Ilmenau) Weimar hall, Large hall

Simulating Coupled Problems on a Million Processor Cores

Ulrich Rüde (Erlangen-Nürnberg)

All modern computer architectures are parallel, not only supercomputers, but even works stations and smart phones. For technological and physical reasons the clock rate of processors cannot be increased further so that only the number of transistors on each chip keeps increasing. In consequence, parallel algorithms are required for all state-of-the-art computing. This is particularly true for demanding coupled systems in science and engineering. We will present two examples. The Earth Mantle is a spherical shell with a volume of a trillion (1012) cubic kilometers. Mantle convection can be modeled by an indefinite finite element problem. We will demonstrate that matrix free parallel multigrid methods can solve such systems with currently up to 1013 (ten trillion) degrees of freedom on almost half a million processor cores in compute times of a few minutes. A second example will be motivated by 3D printing as a modern additive manufacturing technology. We will show how the process can be simulated by a complex combination

of rigid granular dynamics and lattice Boltzmann methods. The scenario involves the generation of a powder bed, controlled energy transfer with an electron beam, melting of the particles, flow of the molten metal, and solidification. With supercomputers, a direct numerical simulation is possible, i.e. representing the physics with full geometric and temporal resolution of each particle and modeling the melt flow subject to surface tension and contact angle conditions.

2 Minisymposia

M 1 : Innovative Discretization Methods, Mechanical and Mathematical Investigations

Tuesday 09:00 - 11:00 Weimar hall, Large hall

Organizers: Stephan Wulfinghoff (Institute of Applied Mechanics, RWTH Aachen University)
Stefanie Reese (Institute of Applied Mechanics, RWTH Aachen University)
Hamid Reza Bayat (RWTH Aachen University)

Reduced integration in IGA at estimated Cauchy-Galerkin points for linear elasticity

F. Fahrendorf (TU Braunschweig, Institut für Angewandte Mechanik), L. De Lorenzis (TU Braunschweig, Institut für Angewandte Mechanik), H. Gomez (Purdue University, School of Mechanical Engineering) 09:00

An efficient implementation of isogeometric analysis (IGA) plays an important rule in current research. Standard Gaussian quadrature rules are not well-suited for an application in IGA, since they do not consider the higher continuity of the shape functions. Therefore different quadrature strategies have been investigated, e.g. in [1, 3, 4, 5, 8]. In addition collocation methods have gained attention, since they have shown to be competitive [7] to Galerkin methods.

Recent improvements regarding the convergence rates of isogeometric collocation methods have been made in [2, 6]. In theses approaches estimates of characteristic evaluation points, named Cauchy-Galerkin points, are used. Collocation at the Cauchy-Galerkin points can reproduce the Galerkin solution exactly, if specific conditions are met. The estimation of these points is based on superconvergence theory. A discrete space constructed by smooth and pointwise non-negative basis functions is required, therefore the approach is convenient for the basis functions typically applied in IGA.

To combine the advantages of the Galerkin and the collocation method, we explore the use of estimated Cauchy-Galerkin points as integration points. Instead of directly using the Galerkin variational formulation of the considered numerical problems, the formulation resulting from an integration by parts is used as a basis for the new quadrature rule. The chosen approach can be seen as an intermediate form between the Galerkin variational formulation and the direct evaluation of the strong form in collocation approaches.

The potential of the method is demonstrated by several numerical examples.

[1] F. Calabrò, G. Sangalli, and M. Tani. *Fast formation of isogeometric Galerkin matrices by weighted quadrature*. arXiv preprint, arXiv:1605.01238, 2016.

[2] H. Gomez and L. De Lorenzis. *The variational collocation method*. Computer Methods in Applied Mechanics and Engineering, 309:152–181, 2016.

[3] R. R. Hiemstra, F. Calabrò, D. Schillinger, and T. J. Hughes. *Optimal and reduced quadrature rules for tensor product and hierarchically refined splines in isogeometric analysis*. Computer Methods in Applied Mechanics and Engineering, preprint, 2016.

[4] T. Hughes, A. Reali, and G. Sangalli. *Efficient quadrature for NURBS-based isogeometric analysis*. Computer Methods in Applied Mechanics and Engineering, 199(5–8):301–313, 2010.

[5] K. A. Johannessen. *Optimal quadrature for univariate and tensor product splines*. Computer Methods in Applied Mechanics and Engineering, preprint, 2016.

[6] M. Montardini, G. Sangalli, and L. Tamellini. *Optimal-order isogeometric collocation at Galerkin superconvergent points*. Computer Methods in Applied Mechanics and Engineering, preprint, 2016.

[7] D. Schillinger, J. Evans, A. Reali, M. Scott, and T. J. R. Hughes. *Isogeometric collocation: Cost comparison with Galerkin methods and extension to adaptive hierarchical NURBS discretizations*. Computer Methods in Applied Mechanics and Engineering, 267:170–232, 2013.

[8] D. Schillinger, S. J. Hossain, and T. J. Hughes. *Reduced Bézier element quadrature rules for quadratic and cubic splines in isogeometric analysis*. Computer Methods in Applied Mechanics and Engineering, 277:1–45, 2014.

A low-order discontinuous Petrov-Galerkin Finite Element Method for linear elasticity

T. Steiner (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), F. Hellwig (Humboldt-Universität zu Berlin, Institut für Mathematik), C. Carstensen (Humboldt-Universität zu Berlin, Institut für Mathematik) 09:20

Standard finite elements with lower order classical Lagrange polynomial shape functions tend to exhibit the phenomenon of volumetric locking for (nearly) incompressible linear elastic materials. The discontinuous Petrov-Galerkin Finite Element Method (dPG-FEM) is introduced to circumvent this locking effect.

The dPG-FEM is a novel mixed method introduced by [1, 2], which was first applied to

wave transport problems and the advection-diffusion-equation. Recently, the dPG-FEM was established for linear elasticity [3]. To obtain the weak form, the balance of linear momentum as well as the constitutive equation are integrated separately and weighted with two distinct test functions. Besides the interpolation of element displacements and stresses, the occuring boundary integrals with displacements and tractions at the interfaces of neighbouring elements are also evaluated. The resulting system of equations contains four primary unknowns, which are discretized with constant ansatz functions for the displacements, stresses and tractions, and linear ansatz functions for the displacements at the interfaces. Furthermore, the two test functions are discretized with linear Lagrangian functions and lowest-order Raviart-Thomas RT_0 functions [4] on the corresponding element leading to a discontinuous formulation. By the choice of different spaces for ansatz and test functions the proposed finite element formulation results in a Petrov-Galerkin scheme.

In the present work a two-dimensional discontinuous Petrov-Galerkin Method with a linear elastic isotropic material model is implemented. The behavior of this formulation is studied with benchmark simulations for small deformations in the nearly incompressible case.

[1] L. Demkowicz, J. Gopalakrishnan: A class of discontinuous Petrov-Galerkin methods. Part I: the transport equation, *Comput. Methods Appl. Mech. Engrg.* 199, 1558–1572, 2010.

[2] L. Demkowicz, J. Gopalakrishnan: A class of discontinuous Petrov-Galerkin methods. Part II: Optimal test functions, *Numer. Methods Partial Differential Equations.* 27 (1), 80–105, 2011.

[3] F. Hellwig, C. Carstensen: Low-Order Discontinuous Petrov-Galerkin Finite Element Methods for Linear Elasticity, *SIAM J. Numer. Anal.* 54 (6), 3388–3410, 2016.

[4] P. A. Raviart, J. M. Thomas: A mixed finite element method for 2-nd order elliptic problems. Mathematical aspects of finite element methods. *Lecture Notes in Mathematics, Springer Verlag New York.* 292–315, 1977.

Stochastic collocation methods for nonlinear probabilistic problems in solid mechanics

J. Rang (TU Braunschweig), H. Matthies (TU Braunschweig) 09:40

In this talk we want to consider stochastic problems in solid mechanics. An conceptionally easy scheme to solve such problems is the Monte Carlo method, where the problems are solved many times with different realisations. But the convergence of the Monte Carlo method is rather slow, needing many solutions of the deterministic problems.

Therefore we consider stochastic methods with a functional approximation. In this case we need a discretisation for the stochastic part which is similar to the spatial discretisation of deterministic PDEs. Moreover the stochastic methods should be implemented in a non-intrusive manner, i.e. the deterministic solver can be used as a block-box.
Therefore we concentrate on stochastic collocation methods, where we introduce a variational framework for the interpolation/approximation method. We apply these methods on some problems in solid mechanics and compare the different approaches.

A phase-field approach to pneumatic fracture

C. Bilgen (University of Siegen, Chair of Solid Mechanics,), R. Krause (Università della Svizzera italiana, Institut of Computational Science), K. Weinberg (University of Siegen, Chair of Solid Mechanics,) 10:00

Phase-field methods for brittle fracture employ a variational framework and have proven to predict complex fracture patterns in two and three dimensional examples. This contribution focuses on a phase-field approach for a coupled field model to brittle and pneumatic fracture in the context of both, finite and linearized strains. Two different challenges are tackled in this talk: First, we have to deal pressure-driven processes within the proposed phase-field ansatz, second, we have to consider the numerical effort of the simulations.
Our phase-field formulation is based on elasticity and a suitable operator split to take only the tensile parts into account. Furthermore, a prescribed pressure is coupled with the phase-field parameter to consider crack propagation induced by pneumatic pressure. We use a semigeometric multigrid method as solution technique for three-dimensional problems to reduce computational complexity. This method employs a pseudo-L^2-projection based prolongation and restriction operators to transfer the information between non-nested meshes. The accuracy and the robustness of the solution method will be demonstrated with a series of numerical examples.

A Monolithic Solution Scheme for a Phase Field Model of Ductile Fracture

T. Noll (University of Kaiserslautern), C. Kuhn (University of Kaiserslautern), R. Müller (University of Kaiserslautern) 10:20

In contrast to conventional sharp crack models, in phase field models cracks are represented by a scalar valued order parameter and thus do not have to be accounted for explicitly in a finite elemnt discretization. The sharp interface between fractured and sound material is described by a smooth transition of the order parameter, characterized by a length parameter. In recent years phase field models for brittle fracture, where the coupling between elastic field and crack field is established by a quadratic degradation function, have become very popular. In order to investigate the impact of plastic deformation on the fracture behavior a plastic contribution can be added. Unlike in the case of brittle fracture no underlying variational formulation exists for the elastic-plastic extension. Depending on the choice of the coupling between the elastic-plastic material law and the order parameter it might become necessary to apply staggered solution schemes.

In this contribution an extension towards quasi static elastic-plastic fracture is presented, where the unaltered conventional radial-return algorithm can be applied and which allows for a monolithic solution scheme to solve the coupled system of equations. Based on numerical examples the crucial role of the degradation function is discussed.

Investigation of a locking-free hybrid discontinuous Galerkin element that is very easy to implement into FE-codes

S. Wulfinghoff (RWTH Aachen University), H. Bayat (RWTH-Aachen University), A. Alipour Kiakalaee (RWTH-Aachen University), S. Reese (RWTH-Aachen University) 10:40

In this work, a hybrid discontinuous Galerkin (dG) quadrilateral element formulation is investigated. As usual in hybrid formulations, the interior of the elements is treated separately from the skeleton, which represents the element boundaries. These are kinematically decoupled, i.e., displacement jumps can occur between skeleton and the interior of the elements. The global degrees of freedom (dofs) are defined on the skeleton as the displacements at the corners, which allows the implementation into existing finite element codes. As usual in hybrid dG-formulations, the dofs in the interior are condensed out on the global level, leading to the same number of global dofs as for continuous bilinear elements.
Instead of using conventional shape function in the interior, the deformation gradient is assumed homogeneous within the element. Furthermore, the deformation gradient is connected to the skeleton degrees of freedom via the weak form. This leads to a very simple formulation and implementation. The element is tested for several computational examples from the literature. Special choices of the penalty parameter are investigated being partially derived analytically. It is found that the element is free of volumetric locking and shear locking. Moreover, the convergence is similar to that of well-known formulations like the Q1E4-, Q1P0- or Q1SP-element.

M 2 : Recent Trends in Phase-Field Modelling

Tuesday 09:00 - 11:00 Weimar hall, Small hall

Organizers: Laura De Lorenzis (TU Braunschweig, Institut für Angewandte Mechanik)
Bernd Markert (RWTH Aachen University)

Variational interface zone model for modeling of fluid induced fracture propagation

I. Khisamitov (Ruhr University Bochum), G. Meschke (Ruhr University Bochum) 09:00

A novel variational framework for aninterface zone model is developed and extended to poroelasticity. As was previously promoted in [1], the total energy of the system is com-

posed by the bulk potential and fracture surface energy. In contrast to the phase-field method [2], the fracture surface is approximated directly along the edges of the finite elements in terms of the interface zero-thickness finite elements. With an introduction of new degree of freedom c (damage field) on the interface level, the solution is found by the minimization of the total potential energy with respect to the displacement and damage fields. An elastic interface constitutive law with the normal and tangential displacement opening formulation is adopted in the pre-fracture regime. Assuming, that a crack propagates according to the Griffith's criterion of brittle fracture, the damage occurs dominantly from the normal opening mode. The Biot's theory is applied both to the bulk and interface elements for the simulation of fluid driven fracture. The pressure field within the interfaces is averaged between the pressures at the bulk element faces. The pressure continuity is enforced by means of a penalty functional. The flow within the fracture is modeled by the cubic law taking the displacement and damage variables into account A number of numerical benchmark tests, which include comparisons with experimental results and analytical solutions, are performed to demonstrate the performance of the model.
Literature [1] B. Bourdin, G.A. Francfort, J.J. Marigo. The variational approach to fracture. J. Elast. 91 (1-3) 2008 5-148. [2] Miehe, C.; Welschinger, F. & Hofacker, M. Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations. International Journal for Numerical Methods in Engineering, John Wiley & Sons, Ltd., 2010, 83, 1273-1311.

Modelling of hydraulic fracturing and fluid flow change in saturated porous domains

Y. Heider (Institute of General Mechanics, RWTH Aachen University), 09:20
B. Markert (Institute of General Mechanics, RWTH Aachen University)

Hydraulic fracturing of porous materials is a challenging but very important subject in various engineering applications, especially in the energy sector. In the man-made enhanced geothermal systems (EGS), which are applied to generate geothermal electricity, high-pressure water is injected into deep rock layers with low permeability in order to enhance the rock's permeability. This leads to improving the system's efficiency and helping to produce electricity with lower prices. Hydraulic fracturing using pressurised liquids with chemical additives is also used in petroleum engineering to extract shale gas. In similar fashion, the developed numerical models can be applied to simulate phenomena like intervertebral disc herniation in biomechanics.
The aim in this research work is to develop a numerical model of fracturing in saturated heterogeneous porous media. To this end, the energy-based phase-field modelling (PFM) scheme together with a proper continuum mechanical approach of multi-phase materials are applied. The proposed modelling framework accounts for the crack nucleation and propagation, deformation of the solid matrix and the different types of fluid flow in the porous domain and the crack, see [1, 2] for details and references. In particular, the material description of the fluid-saturated porous materials is based on the theory of porous media (TPM). The proposed treatment assumes a steady-state behaviour (quasi-

static) and neglects all thermal and chemical effects as well as any mass exchange between the constituents. Special focus is on the description of the interface between the porous domain and the free flow in the crack. To reveal the ability of the proposed modelling strategy in capturing the basic features of hydraulic fracturing, numerical examples using the finite element method will be presented and compared with experimental data.

[1] Markert, B., Heider, Y.:*Coupled Multi-Field Continuum Methods for Porous Media Fracture, in: Recent Trends in Computational Engineering - CE2014*, Vol. 105 of Lecture Notes in Computational Science and Engineering. Springer International Publishing, pp.167–180 (2015).

[2] Heider, Y., Markert, B.: *A phase-field modeling approach of hydraulic fracture in saturated porous media*, Mech. Res. Commun., DOI:10.1016/j.mechrescom.2016.07.002 (2016).

Phase-field modeling of fracture in partially saturated porous media

T. Cajuhi (Technische Universität Braunschweig), L. Sanavia (University of Padova), L. De Lorenzis (Technische Universität Braunschweig) 09:40

Porous media such as soil, rocks and concrete are of great importance in the context of civil engineering and environmental geomechanics. They consist of a solid skeleton and pores filled with fluids, e.g. air and water. Complex mechanisms of flow and transport take place within the pore network and can lead to deformation of the solid skeleton and eventually to fracture phenomena [1]. Phase-field modeling of fracture has recently emerged as an alternative to conventional approaches such as remeshing, extended finite element methods or cohesive zone modeling. The phase-field framework can be considered a special type of gradient damage modeling approach, where a diffusive approximation of the crack is taken into account and the continuous phase-field parameter is used to describe the material integrity. The essential advantages are the possibility to describe arbitrarily complicated fracture patterns such as nucleation, branching and merging, without ad-hoc criteria on a fixed mesh, through the solution of partial differential equations derived from variational principles [2-5]. Phase-field modeling of fracture in porous media has been addressed in some recent publications [6-7], which however have only focused on the fully saturated case. Objective of this contribution is to describe fracture in partially saturated porous media using a phase-field approach. In this study, the material is described by its linear-elastic properties. The overall balance of linear momentum, the continuity equation and the phase-field evolution equation constitute a nonlinear coupled and time-dependent system of equations, which needs to be discretized and linearized. We formulate the coupled non-linear system of partial differential equations governing the problem with displacements, capillary pressure and crack phase-field as unknowns. The spatial discretization is carried out with finite elements of appropriate order for the different unknowns. We discuss its solution and present some relevant examples.

Keywords: porous media, fracture, phase-field modelling.

[1] L. Simoni, B.A. Schrefler, Multi field simulation of fracture. Advances in Applied Mechanics, 2014.

[2] B. Bourdin, G.A. Francfort, J-J. Marigo, Numerical experiments in revisited brittle fracture. Journal of the Mechanics and Physics of Solids, 48, 797-826, 2000.
[3] C. Miehe , F. Welschinger, M. Hofacker, Thermodynamically consistent phase-field models of fracture: variational principles and multi-field FE implementations. International Journal for Numerical Methods in Engineering, 83, 1273-1311, 2010.
[4] C. Kuhn, R. Muller, A continuum phase field model for fracture. Engineering Fracture Mechanics 77, 3625-3634, 2010.
[5] M. Ambati, T. Gerasimov, L. De Lorenzis, A review on phase-field models of brittle fracture and a new fast hybrid formulation. Computational Mechanics 55, 383-405, 2014.
[6] A. Mikelić, M.F. Wheeler, T. Wick, A phase-field method for propagating fluid-filled fractures coupled to a surrounding porous medium. SIAM Multiscale Modeling and Simulation 13(1), 367-398, 2014.
[7] A. Mikelić, M.F. Wheeler, T. Wick, Phase-field modeling of a fluid-driven fracture in a poroelastic medium. Computational Geosciences pp. 1-25, 2015.

Phase Field Models for the Failure of Anisotropic Continuum

H. Dal (Middle East Technical University), O. Gültekin (Graz University of Technology), F. Denli (Middle East Technical University), G. Holzapfel (Graz University of Technology) 10:00

This study presents a phase-field approach for an anisotropic continuum to model fracture of biological tissues and fibre-reinforced composites. We start by deriving the regularized crack surface to overcome complexities inherent in sharp crack discontinuities, thereby relaxing the acute crack surface topology into a diffusive one. In fact, the regularized crack surface possesses the property of Gamma-Convergence, i.e. the sharp crack topology is restored with a vanishing length-scale parameter. Next, we deal with the continuous formulation of the variational principle for the multi-field problem manifested through the deformation map and the crack phase-field at finite strains which leads to the Euler–Lagrange equations of the coupled problem. In particular, the coupled balance equations derived render the evolution of the anisotropic crack phase-field and the balance of linear momentum. As an important aspect of the continuum formulation we consider an invariant-based anisotropic constitutive models for single and multiple families of fibers embedded in the ground matrix. In addition we propose a novel energy-based anisotropic failure criterion which regulates the evolution of the crack phase-field. The coupled problem is solved using a one-pass operator-splitting algorithm composed of a mechanical predictor step and a crack evolution step. Various anisotropic failure criteria are studied. Our preliminary investigations suggest that the novel energy based anisotropic failure criteria presented is superior to stress based criteria existing in the literature. Representative numerical examples are devised for crack initiation and propagation in CFRP composites and rupture in thoracic aorta. Model parameters are obtained by fitting the set of novel experimental data to the predicted model response; the finite element results agree favorably with the experimental findings.

O. Gültekin, H. Dal, and G. A. Holzapfel. A phase-field approach to model fracture of arterial walls: Theory and finite element analysis *Comput. Meth. Appl. Mech. Eng.*, 312:542–566, 2016.

O. Gültekin, H. Dal, and G. A. Holzapfel. Numerical Aspects of Failure in Soft Biological Tissues Favor Energy-based Criteria: A Rate-dependent Mixed Crack Phase-field Model *Comput. Meth. Appl. Mech. Eng.*, under review.

F. Denli, O. Gültekin, and H. Dal. An Anisotropic phase-field model for polymers Part I: Quasi-static small strain formulation for CFRP composites *Int. J. Numer. Meth. Engng.*, in preparation

Phase-field description of fracture in plates and shells

M. Ambati (TU Braunschweig, Institut für Angewandte Mechanik), J. Kiendl (Norwegian University of Science and Technology, Department of Marine Technology), L. De Lorenzis (TU Braunschweig, Institut für Angewandte Mechanik), H. Gomez (University of Coruna, Department of Mathematical Methods and Representation), A. Reali (University of Pavia, Department of Civil Engineering and Architecture) 10:20

Phase-field modeling of brittle fracture is a modern promising approach that enables a unified description of complicated failure processes (including crack initiation, propagation, branching, merging), as well as its efficient numerical treatment. In this work, we apply this approach to model fracture in thin structures like plates and shells. The kinematics and the phase field are defined on the midsurface of the structure. Here, brittle fracture and a Kirchhoff-Love (KL) shell model for structural analysis are considered. It is shown that the variation of strains through the shell thickness has to be considered and the split into tensile and compressive elastic energy components, needed to prevent cracking in compression, has to be carried out at various points through the thickness, which prohibits the typical separation of the elastic energy into membrane and bending terms. In this case, a rotation-free KL shell model developed by Kiendl et al. [1]-[2] is combined with phase-field brittle fracture description. A careful investigation on various numerical examples under different possible strain states and detailed comparisons with three dimensional solid simulations are carried out to confirm the accuracy and efficiency of the proposed model.

[1] J. Kiendl, K.-U. Bletzinger, J. Linhard, R. Wüchner (2009). Isogeometric shell analysis with Kirchhoff-Love elements. Computer Methods in Applied Mechanics and Engineering 198:3902–3914.

[2] J. Kiendl, M.C. Hsu, M.C.H. Wu, A. Reali (2015) Isogeometric Kirchhoff-Love shell formulations for general hyperelastic materials. Computer Methods in Applied Mechanics and Engineering 291:280–303.

Modelling of the gelation process of biopolymers using phase-field method

B. Zhou (Institute of General Mechanics), Y. Heider (Institute of General Mechanics), B. Markert (Institute of General Mechanics) 10:40

Biopolymer gels have many applications in tissue engineering. In recent years, biopolymer gels are widely used as scaffold material in the three dimensional bioprinting technique for tissues and organs. To optimize the printing process, it becomes important to study and understand the temperature- and time- dependent gelation kinetics of biopolymer gels [1].

In this study, a thermodynamic model is proposed to describe the gelation kinetics of thermoreversible gels, which are driven by coil-to-helix transition [2]. In this model, the gelation process is assumed to proceed in two steps. The process starts from the reference state, in which the solution consists of solvent molecules and polymer chains with n segments in random coil configuration. Polymer chains firstly change from the random coil state to the partially helical state, followed by the aggregation of helical parts of polymer chains. This formation and the followed aggregation of helices lead to the eventual polymer network. A parameter ϕ is employed to describe the volume fraction of polymers which belong to the network. It also represents the degree of gelation. The free energy density is calculated based on the Flory Huggins theory and the statistics model of coil-to-helix transition.

With the help of the phase-field method, see [3], numerical simulations of a spatial and time varied gelation process of droplets in 3D Bioprinting are performed using the finite element method.

[1] Zhou, B. and Heider, Y. and Blaeser, A. and Raith, S. and Fischer, H. and Markert, B.: *Simulation of the gelation process of hydrogel droplets in 3D bioprinting*, Vol. 16 of PAMM, pp. 117–118 (2016).

[2] Tanaka, F.: *Thermoreversible gelation driven by coil-to-helix transition of polymers*, Vol. 36 of Macromelecules, pp. 5392–5405 (2003).

[3] Boettinger, W. J. and Warren, J. A. and Beckermann, C. and Karma, A.: *Phase-field simulation of solidification*, Vol. 32 of Annual Review of Materials Science, pp. 163–194 (2002).

M 3 : Dislocation-based Plasticity: State of the Art and Challenges

Tuesday 09:00 - 11:00 Weimar hall, Seminar room 1

Organizers: Eric Bayerschen (Karlsruher Institut für Technologie (KIT))
Thomas Böhlke (Karlsruher Institut für Technologie (KIT))
Katrin Schulz (Karlsruhe Institute of Technology (KIT))

Computational and theoretical aspects of a grain-boundary model that accounts for grain misorientation and grain-boundary orientation

A. McBride (University of Glasgow), D. Gottschalk, D. Reddy, P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 09:00

The miniaturisation of mechanical components composed of crystalline material requires a continuum theory that accounts for the role of the grain boundary and for size-dependent effects. The grain-boundary model should incorporate both the *misorientation in the crystal lattice* between adjacent grains, and the *orientation of the grain boundary* relative to the crystal lattice of the adjacent grains. Classical theories of plasticity are unable to describe the well-known size-dependent response exhibited by crystalline material at the micro- and nanometre scale. Numerous extended (gradient and non-local) continuum theories of single-crystal plasticity have been presented in the last two decades to circumvent these limitations.
The aim of this presentation is to summarise a recent theoretical and numerical investigation of the infinitesimal single-crystal gradient-plasticity and grain-boundary theory of Gurtin (2008). The governing equations and flow laws are recast in variational form. The associated incremental problem is formulated in minimization form and provides the basis for the subsequent finite element formulation. Various choices of the kinematic measure used to characterize the ability of the grain boundary to impede the flow of dislocations are compared. A series of three-dimensional numerical examples serve to elucidate the theory.

Development of dislocation density based constitutive models - the parameter dilemma

F. Roters (MPI für Eisenforschung GmbH), M. Bambach (BTU Cottbus - Senftenberg), S. Wong (MPI für Eisenforschung GmbH) 09:20

The key problem of empirical constitutive models is the fact that in general we do not know anything about the parameters involved, i.e. the parameters can have any arbitrary value. Also empirical models cannot be improved in a systematic way. It is, however, often claimed that these problems can be overcome by the use of physics based models. Dislocation density based models for plastic deformation are one example for such physics based models. They can be systematically extended by taking more dislocation processes into account and by a better discretization of the dislocation densities themselves. Also as most parameters have a physical meaning their values are known, which makes the

determination of the remaining fitting parameters much easier. But is this really true? Unfortunately not! Mostly only the order of magnitude for the parameter values is known and in the end a large number of them needs to be fitted to experimental data. The talk discusses this questions and shows examples how lower scale models can help reducing the number of fitting parameters and thus finding the desired unique parameter set.

A canonical rate-independent model of geometrically linear isotropic gradient plasticity with isotropic hardening and plastic spin accounting for Burgers vector

P. Neff (University of Duisburg-Essen), F. Ebobisse, K. Hackl (Institute of Mechanics of Materials, Ruhr-Universität Bochum) 09:40

In this work we propose a canonical variational framework for rate-independent phenomenological geometrically linear gradient plasticity with plastic spin. The model combines the additive decomposition of the total distortion into non-symmetric elastic and plastic distortions, with a defect energy contribution taking account of the Burgers vector through a dependence only on the dislocation density tensor Curl p giving rise to a non-symmetric nonlocal backstress, and isotropic hardening response only depending on the accumulated equivalent plastic strain. The model is fully isotropic and satisfies linearized gauge-invariance conditions, i.e., only true state-variables appear. The model satisfies also the principle of maximum dissipation which allows to show existence for the weak formulation. For this result, a recently introduced Korn's inequality for incompatible tensor fields is necessary. Uniqueness is shown in the class of strong solutions. For vanishing energetic length-scale, the model reduces to classical elasto-plasticity with symmetric plastic strain and standard isotropic hardening.

A mechanism-based homogenization strategy for the determination of flow stress and strain hardening

K. Schulz (KIT Karlsruher Institut für Technologie), M. Sudmanns, P. Gumbsch (Karlsruher Institut für Technologie) 10:00

Metal forming simulations today are based on classical constitutive descriptions of yield behavior and hardening. Microstructural materials characteristics like grain size or dislocation microstructure are rarely considered and never systematically evolved. In the last years, the striving for advanced materials with well-defined microstructures has led to an increasing effort towards a physically based description of plastic deformation processes. However, small-scale approaches which include the microstructure of defects of the material in a discrete way come along with the drawback of very high computational costs. Based on the evolution of dislocation densities in a continuum model, we introduce an efficient numerical strategy for representing the evolution processes as well as the dislocation interactions in a material. Herein, a fully three dimensional set-up is considered, representing the elasto-plastic deformation processes in face centered cubic crystals. The issue of the transition between a discrete and a continuous representations of dislocation microstructures is addressed as a central question.

Single-crystal gradient plasticity with application to oligocrystals

T. Böhlke (Karlsruher Institut für Technologie), E. Bayerschen (Karlsruher Institut für Technologie), A. Prahs (Karlsruher Institut für Technologie) 10:20

A geometrically linear gradient plasticity (GP) model is presented. It includes a phenomenological grain boundary (GB) yield condition [1] to model the resistance of GBs against plastic flow. The theory is implemented with finite elements. Comparison of GP simulations to discrete dislocation dynamics (DDD) simulations are performed [2] motivating an extension of the GB yield strength with a hardening term [2,3]. Remaining discrepancies in the plastic strain gradients motivate substituting the quadratic defect energy of the GP framework by a generalized defect energy [4].
Recently, contrary size effects have been observed in experiments on thin gold wires under tensile and torsion loading [5]. Finite element simulations of simplified grain aggregates are performed to simulate the mechanical response of the wires. Emphasis is put on the interpretation and understanding of the size effects. It is shown, that accounting for the wire texture is of central importance in explaining the contrary size effects under different loading conditions [6].
The presentation of physically based model enhancements, e.g., full coupling [7] of the geometrically linear GP model to CDD theory [8], and the consideration of orientation-dependent grain boundary mechanisms complete this talk.

[1] Wulfinghoff, S., Bayerschen E., Böhlke, T. (2013). Int. J. Plast. 51, 33-46.
[2] Bayerschen, E., Stricker, M., Wulfinghoff, S., Weygand, D., Böhlke, T. (2015). Proc. R. Soc. A 2015, 471, 20150388
[3] Bayerschen, E., Stricker, M., Weygand, D. and Böhlke, T. (2016). Proc. Appl. Math. Mech., 16: 301-302.
[4] Bayerschen, E. & Böhlke, T. (2016). Comput. Mech. 58: 13.
[5] Chen Y., Kraft O., Walter M. (2015). Acta Mater. 87:78-85.
[6] Bayerschen, E., Prahs, A., Wulfinghoff, S., Ziemann, M., Gruber, P. A., Walter, M., Böhlke, T. (2016). J. Mater. Sci. 51: 7451-7470.
[7] Wulfinghoff, S., Böhlke, T. (2015). Int. J. Plast., 69, 152-169.
[8] Hochrainer, T. , Sandfeld, S., Zaiser, M., Gumbsch, P. (2014). J. Mech. Phys. Solids, 63, 167-178

Numerical approximation of a mesoscale approach for the dislocation density evolution in crystal plasticity

C. Wieners (KIT), L. Wagner 10:40

Classical macroscopic approaches in continuum mechanics for single crystal plasticity fail to describe the physical mechanisms induced by dislocation motion. On the other hand, small-scale approaches directly simulating single dislocations require extremely high computational costs. Here, we consider a mesoscale model for the evolution of dislocation densities based on small-strain single-crystal plasticity combined with Orowan's relation for the plastic shear strain in every slip system of the crystal. The system is

closed by an evolution system for averaged dislocation densities and dislocation curvature densities (derived from the higher order continuum dislocation theory developed by Hochrainer et al.) and a constitutive law for the dislocation velocity. We introduce a fully coupled numerical method combining a conforming finite element approximation of elasto-plasticity with an implicit Runge-Kutta discontinuous Galerkin discretization of the dislocation system which allows for 3D computations including multiple slip systems and dislocation interaction.

M 4 : Nonlinear Approximations for High-dimensional Problems

Tuesday 09:00 - 11:00 Weimar hall, Seminar room 4

Organizers: Markus Bachmayr (Universität Bonn)
Ivan Oseledets

Nonlinear multilevel approximation of functions by tensor structure

V. Kazeev (University of Geneva) 09:00

Tensor decompositions, separating variables in high-dimensional arrays, are mostly seen as an efficient tool for lifting the so-called "curse of dimensionality" in high-dimensional settings. In such cases, polynomial approximations are often used in the "physical" and, possibly, parametric spaces to translate a continuous problem into a discrete (tensor) problem. Such approximations are however known to converge slowly when the solution has low regularity or when the regularity constants are prohibitively large, which is the case for singular and highly oscillatory solutions. This poses a challenge even in low dimensions. Many discretizations have been developed for such problems, such as the adaptive *hp*-FEM and the heterogeneous multiscale method.
When applied to resolve the multiscale structure of the data, a tensor decomposition may be expected to realize the efficient representation of solutions while retaining a standard, problem-nonspecific discretization scheme based on tensor-product grids and low-order approximation. Recently, the so-called quantized-tensor-train (QTT) decomposition has been shown to achieve exponential convergence (with respect to the number of effective degrees of freedom) in certain problems with singular and highly oscillatory solutions. These convergence results build, in particular, upon the tensor-rank bound for the polynomial functions by Grasedyck. This talk elaborates on the interpretation of the QTT decomposition as a function-approximation framework and presents refined bounds for the QTT approximation of polynomial and piecewise-analytic functions.

On the approximation of electronic wavefunctions by anisotropic Gauss and Gauss-Hermite functions

S. Scholz (Technische Universität Berlin), H. Yserentant (Technische Universität Berlin) 09:20

The electronic Schrödinger equation describes the motion of N electrons under Coulomb

interaction forces in a field of clamped nuclei. The solutions of this equation, the electronic wavefunctions, depend on $3N$ variables, three spatial dimensions for each electron. We study the approximability of these wavefunctions by linear combinations of anisotropic Gauss functions, or more precisely Gauss-Hermite functions, products of polynomials and anisotropic Gauss functions in the narrow sense. We show that the original, singular wavefunctions can up to given accuracy and a negligibly small residual error be approximated with only insignificantly more such terms than their convolution with a Gaussian kernel of sufficiently small width and that basically arbitrary orders of convergence can be reached.

Block eigensolvers on low-rank tensor manifolds

M. Rakhuba (Skolkovo Institute of Science and Technology) 09:40

In this work we focus on a solution of symmetric eigenvalue problems with eigenvectors that admit a low-rank representation in the Tensor Train (TT) format. The straightforward extension of iterative methods, e.g. locally-optimal block preconditioned conjugate gradient method (LOBPCG), leads to the instability and/or to the rank growth. Alternatively one can solve an eigenvalue problem as an optimization procedure in the block tensor format, which is time-consuming when a large number of eigenvectors is to be found.
To resolve these problems we exploit a priori information that eigenvectors can be represented in the TT-fromat in the following way. We propose [1] to use well-established iterative methods that utilize matrix inversion (e.g. LOBPCG, inverse iteration) and solve corresponding linear systems inexactly along the manifold of low-rank tensors to accelerate the convergence.
As an application, we accurately compute 100 eigenvectors and eigenvalues of a realistic Hamiltonian.

[1] Maxim Rakhuba and Ivan Oseledets. *Calculating vibrational spectra of molecules using tensor train decomposition.* J. Chem. Phys., pages 124101, 2016. doi:10.1063/1.4962420

Labelled Modes - A New Notation for Tensor Networks

S. Etter (University of Warwick) 10:00

When writing about tensor networks, authors frequently face the challenge of balancing generality, precision and conciseness of the exposition. Intending to abolish the need for such compromises, I will present a new notation which allows to discuss general tensor networks with a notational simplicity comparable to that of the most prominent special case, tensor trains, but is nevertheless perfectly precise such that it allows for word-by-word translation into computer code. The notation's key feature is that it assigns a global identity to the tensor modes, unlike existing notations where modes can only be addressed as parts of the tensor in which they appear. This talk will present several

examples to demonstrate that introducing such *labelled modes* simplifies the formulae and leads to code which is both easier to write as well as to debug.

On the Expressive Power of Deep Learning: A Tensor Analysis

N. Cohen (The Hebrew University of Jerusalem) 10:20

We derive an equivalence between convolutional networks – the most successful deep learning architecture to date, and tensor decompositions. The equivalence is used to analyze the expressive properties of such networks, settling old conjectures as well as proving new and surprising results. We show that with linear activation and product pooling, almost all functions realized by a deep network require exponential size in order to be realized (or approximated) by a shallow network. Surprisingly, the result no longer holds when the activation and pooling operators are switched to ReLU and max/average respectively. This suggests that in terms of expressiveness, the most popular type of convolutional networks is inferior to an alternative "arithmetic circuit" variant, which has recently been implemented and is showing promising results in practice. We focus on the latter, extending the analysis beyond separation of depths. Specifically, we study expressible functions in terms of their ability to model correlation between regions of the input. We find that this ability is only achievable through depth, and that a deep network's pooling geometry selects which correlations can be modeled, thereby controlling the inductive bias. Contiguous pooling windows as commonly employed in practice favor correlations between interleaved regions, orienting the inductive bias towards the statistics of natural images. Other pooling schemes lead to different preferences, and this allows tailoring the network to data that departs from the usual domain of natural imagery.

M 5 : Structured Preudospectra and Stability Radii: Applications and Computational Issues

Tuesday 09:00 - 11:00 Coudraystr. 11C, Lecture hall 1

Organizers: Nicola Guglielmi (University of L'Aquila)
Michael Karow (TU Berlin)

Approximating the Real Structured Stability Radius with Frobenius Norm Bounded Perturbations

N. Guglielmi (Università dell'Aquila), M. Gürbüzbalaban (Rutgers University), T. Mitchell (Max Planck Institute for Dynamics of Complex Technical Systems), M. Overton (New York University) 09:00

We propose a fast method to approximate the real stability radius of a linear dynamical system with output feedback, where the perturbations are restricted to be real valued and bounded with respect to the Frobenius norm. Our work builds on a number of scalable algorithms that have been proposed in recent years, ranging from methods

that approximate the complex or real pseudospectral abscissa and radius of large sparse matrices (and generalizations of these methods for pseudospectra to spectral value sets) to algorithms for approximating the complex stability radius (the reciprocal of the H_∞ norm). Although our algorithm is guaranteed to find only upper bounds to the real stability radius, it seems quite effective in practice. As far as we know, this is the first algorithm that addresses the Frobenius-norm version of this problem. Because the cost mainly consists of computing the eigenvalue with maximal real part for continuous-time systems (or modulus for discrete-time systems) of a sequence of matrices, our algorithm remains very efficient for large-scale systems provided that the system matrices are sparse.

Local structured perturbation of eigenvalues of symplectic matrices: a multiplicative approach

J. Moro (Universidad Carlos III de Madrid), F. Sosa (Universidad Carlos III de Madrid), C. Mehl (Technische Universität Berlin) 09:40

Small structured eigenvalue perturbations of symplectic matrices are analyzed via Newton diagram techniques by modelling perturbations multiplicatively: any symplectic perturbation $\widehat{S}$ of a symplectic matrix S is written as $\widehat{S} = (I + \epsilon B + O(\epsilon^2))S$, with B Hamiltonian. This allows to make use of the first order multiplicative perturbation theory developed in [2] to obtain both leading exponents and explicit formulas for the leading coefficients in the eigenvalue asymptotic expansions.

Thecorresponding analysis requires using symplectic structured canonical forms to give a very detailed description of the connections between left and right eigenvectors induced by symplectic structure. In most cases, provided some mild genericity conditions are met, only the perturbation matrix B and appropriately normalized eigenvectors (i.e., no generalized eigenvectors) are involved in the formulas.

For rank one perturbations, these results are a complement to those in [1], wherethe generic change in the perturbed Jordan canonical form under rank-one structured symplectic perturbation is characterized. The asymptotic expansions above describe the local perturbation behavior of the new eigenvalues originated fromthose Jordan blocks destroyed by the structured perturbation, as predicted in [1]. However, it should be noted that the first order perturbation expansions are valid for perturbations of *any* rank.

[1] C. Mehl, V. Mehrmann, A. C. Ran and L. Rodman, *Eigenvalue perturbation theory of structured matrices under generic structured rank one perturbations: Symplectic, orthogonal, and unitary matrices*, BIT Numer. Math., Vol. 54 , 2014, pp. 219–255.

[2] F. Sosa & J. Moro, *First order asymptotic expansions for eigenvalues of multiplicatively perturbed matrices*, SIAM J. Matrix Anal. Appl., Vol. 37 no. 4, 2016, pp. 1478–1504.

Real structured distance to instability for linear Hamiltonian systems with perturbed dissipation

P. Sharma (University of Mons), V. Mehrmann, C. Mehl 10:20

Linear dissipative-Hamiltonian (DH) systems with real constant coefficients arise in energy based modeling of dynamical systems. Making use of the structure, they are automatically stable. However, they are not in general asymptotically stable. It is important to know that when a real linear constant coefficient DH system is on the boundary of the region of asymptotic stability, i.e. when it has purely imaginary eigenvalues, or how much it has to be perturbed to be on this boundary. For unstructured systems this *real distance to instability (real stability radius)* has been a challenging problem.
We analyze this real distance under different structured perturbations to the dissipation term that preserve the DH structure. We derive explicit formulas for this distance in terms of low rank perturbations. The results are illustrated by numerical experiments. These show that the DH system is much more robustly stable under real structured perturbations to the dissipation than for unstructured perturbations. We also compare the real stability radius with its complex counterpart recently studied in [1]

[1] C. Mehl, V. Mehrmann and P. Sharma. Structured distances to instability for linear Hamiltonian systems with dissipation. *SIAM Journal on Matrix Analysis and Applications*, 37:4, 1625-1654., 2016.

M 6 : Turbulent Liquid Metal and Magnetohydrodynamic Flows

Tuesday 09:00 - 11:00 Coudraystr. 13A, 1st floor, Lecture hall 2
Organizers: Leo Bühler (Karlsruhe Institute of Technology (KIT))
Jörg Schumacher (TU Ilmenau, Fak. Maschinenbau)

Heated vertical duct flow of liquid metal with and without expansion

M. Niemann (Technische Universität Dresden), J. Fröhlich (Technische Universität Dresden) 09:00

The effects of buoyancy on vertical duct flows with one heated side wall are investigated by means of Direct Numerical Simulations. In particular, the flow through square ducts and behind the expansion of a wide backward-facing step are presented and results at several Reynolds and Richardson numbers are considered in the forced and mixed convection regime. For all configurations one wall is heated and all other side walls are treated as adiabatic. These configurations allow studying the interaction of buoyancy forces and, on the one hand, the secondary flow in the square duct and, on the other hand, with the shear layer and recirculation zone behind the expansion.
In both configurations, buoyancy substantially alters the mean flow field and, consequently, turbulent stresses and heat transfer compared to the forced convection cases.

This contribution will give an overview of these alterations and quantify the enhancement of heat transfer and turbulence with Richardson and Reynolds number. Behind the step this is mainly because buoyancy precipitates reattachment and thus attenuates the recirculation zone which obstructs heat transfer in the forced convection case. For the square duct, secondary flow of the second kind is present due to the side walls and interacts with the buoyancy forces. This interaction has an additional and substantial impact on turbulence and heat transfer. Budgets of turbulent kinetic energy, Reynolds stresses, temperature variance, and turbulent heat fluxes are available for all investigated cases. These budgets give valuable insight into the interactions of the particular fields and are useful references for modeling turbulent heat transfer in liquid metal flows in the forced as well as in the mixed convection regime.

Turbulent liquid metal heat transfer in rod bundles

A. Class (Karlsruhe Institute of Technology (KIT)), K. Litfin (Karlsruhe Institute of Technology (KIT)), J. Pacio (Karlsruhe Institute of Technology (KIT)), T. Wetzel (Karlsruhe Institute of Technology (KIT)) 09:20

Heavy liquid metals (HLM) are prominent coolant candidates for advanced nuclear reactors and target material of spallation sources. The Karlsruhe liquid metal laboratory (KALLA) performs fundamental thermal hydraulic studies up to component scale. In this framework different rod-bundle designs have been investigated to support the design and licensing of the Multi-purpose hybrid research reactor for high-tech applications (MYRRHA) facility to be built in Mol, Belgium. The growing complexity from single heated rod, via spacer and wire grid 19-pin rod bundles to multiple connected rod bundle geometries is covered in an ongoing series of experiments starting in 2004. Data acquisition by local high speed temperature measurements at up to 40 different positions within the rod bundle gives an insight into turbulent heat transfer in the complex structure. Pre test analysis by CFD is performed to optimize the experimental setup as well as measurement positions. Post test analysis allows to verify and validate the applied models for turbulent flow and heat transfer.

Magnetohydrodynamic flows in liquid metal blankets for fusion reactors

C. Mistrangelo (Karlsruhe Institute of Technology (KIT)), L. Bühler (Karlsruhe Institute of Technology (KIT)) 09:40

Liquid metal blankets are proposed to be tested in the experimental fusion reactor ITER. Three main concepts are currently under development. In the water cooled and in the helium cooled lead lithium blankets the PbLi alloy serves as breeder material for producing the fuel component tritium used in the magnetically confined fusion plasma. The generated fusion heat is efficiently removed by a separated water or helium cooling system and therefore the liquid-metal could be practically at rest. However, for tritium extraction in external ancillary systems a weak circulation (1 mm/s) is required. In the dual coolant lead lithium blanket the liquid metal serves both to produce tritium and to remove the volumetric heat deposited in the breeding zone (BZ), while helium is employed to cool first wall and blanket structure. In this concept PbLi has to flow

faster (1 cm/s) than in the separately cooled blanket designs to allow efficient cooling of the BZ. In liquid metal blankets there are common issues related to the specific characteristics of the liquid metal. The interaction of the electrically conducting fluid with the strong confining magnetic field induces electric currents and electromagnetic forces that influence velocity and pressure distribution. Lorentz forces are balanced by pressure gradients and this results in increased pressure drop compared to hydrodynamic conditions. These additional pressure losses are proportional to the electric current density induced in the fluid. By electrically decoupling PbLi and the conducting walls, for instance by means of insulating channel inserts, the total current density and related pressure drop reduce. Other MHD phenomena that have to be taken into account are complex magneto-convective flow patterns, electrical coupling of adjacent fluid domains that results from the presence of leakage currents crossing common conducting walls. Such a coupling can lead to reversed flow in some regions of blanket modules and non-uniform flow partitioning in parallel ducts. The described MHD phenomena are present in all liquid metal blankets, but their impact on the system performance is concept-specific.

Properties of turbulent and transitional electromagnetic boundary layers in channels with a uniform magnetic field

D. Krasnov (TU Ilmenau), L. Braiden (Coventry University), L. Bühler (Karlsruher Institut für Technologie), S. Molokov (Coventry University), O. Zikanov (University of Michigan - Dearborn), T. Boeck (TU Ilmenau) 10:00

Liquid metal flows in the presence of a uniform magnetic field experience electromagnetic induction. The eddy currents and associated Lorentz force density modify the flow and give rise to thin electromagnetic boundary layers on the walls of the channel or duct. Hartmann layers develop on the walls perpendicular to the magnetic field whereas side layers develop on the parallel walls. The structure of the laminar flow depends on the conductivity of the walls. The side layers play a critical role in the transition to turbulence and are also strongly affected by the anisotropic character of the Lorentz force. We report numerical studies of duct flows with insulating and conducting Hartmann walls covering transitional and turbulent regimes. We point out the differences between these cases and analyze the mean properties as well as specific transitional patterns. Simple models for the turbulent mean flow are also reviewed and compared to the data obtained in high-resolution direct numerical simulations.

The DRESDYN project: planned experiments and present status

F. Stefani (Helmholtz-Zentrum Dresden-Rossendorf), S. Eckert, G. Gerbeth, A. Giesecke, T. Gundrum, D. Räbiger, M. Seilmayer, T. Weier 10:20

The Dresden sodium facility for dynamo and thermohydraulic studies (DRESDYN) is a platform for large-scale liquid sodium experiments devoted both to fundamantal geo- and astrophysical questions as well as to various applied problems related to the conversion and storage of energy. Its most ambitious part is a precession driven dynamo experiment, comprising 8 tons of liquid sodium supposed to rotate with up to 10 Hz and to precess

with up to 1 Hz. Another large-scale set-up is a Tayler-Couette experiment with a gap width of 0.2 m and a height of 2 m, whose inner cylinder rotates with with up to 20 Hz which provides a magnetic Reynolds number of about 40. Equipped with a coil system for the generation of an axial field of up to 120 mT (giving a Lundquist number of around 40) and two different axial currents through the center and the liquid sodium, this experiment aims at studying various versions of the magnetorotational instability and their combinations with the Tayler instability. The lecture will focus on the physical background of these two experiments, but will also delineate the present status of their technical realization. Other installations, such as a sodium loop and a test stand for liquid metal batteries, will also be sketched.

Local Lorentz force velocimetry at a continuous casting model

D. Hernández (Technische Universität Ilmenau), C. Karcher (Technische Universität Ilmenau), T. Wondrak (Helmholtz-Zentrum Dresden-Rossendorf) 10:40

Local Lorentz force velocimetry is a local velocity measurement technique for liquid metals. Due to the interaction between an electrically conductive liquid and an applied magnetic field, eddy currents and flow-braking Lorentz forces are induced within the fluid. Due to Newton's third law, a force of the same magnitude acts on the source of the applied magnetic field, which is in our case a permanent magnet. The magnet is attached to a force/torque sensor that has been especially developed to record all three force and three torque components acting on the magnet. This new-generation local Lorentz force flowmeter (L2F2) has already been tested at a test stand for continuous casting with a 15 mm cubic magnet providing an insight into the three-dimensional velocity distribution of the model melt GaInSn near the wide face of the mold. However, the torque component perpendicular to this surface was not accessible at all. In the present paper, we describe the numerical model and the corresponding results that show that with a cross-shaped magnet we are able to measure this torque in liquid metals using our sensor. According to our results, this torque correlates with the curl of the velocity in this direction.

M 7 : Flow Separation and Vortical Phenomena: Simulation in Progress

Tuesday 09:00 - 11:00 Weimar hall, Seminar room 3

Organizers: Markus Rütten (German Aerospace Center (DLR) - Institute of Aerodynamics and Flow Technology)
Wolfgang Schröder (RWTH Aachen University)

Challenges and applications of overset grid coupling strategies

S. Völkner (TUHH), T. Rung 09:20

Overset grid methods offer a common approach for the simulation of complex flows

featuring dynamically moving geometries and large relative motion [1, 2]. In combination with incompressible finite-volume methods, which employ a co-located and cell-centred variable arrangement, overset grid methods have to be treated with caution, since the local interpolation of field values onto the partner grids [3] violates the inherent mass conservation of the finite-volume approach. As the mass defect directly influences the pressure solution, the interpolation-induced mass imbalance can result in severe pressure fluctuations when mass conservation is not enforced. The particular interest is to show the influence of different interpolation schemes and present mass conservation practices [2, 4], which have been successfully applied on unstructured three-dimensional grids.
Further challenges deal with HPC using dynamic load balancing and the restriction of a sufficient overlap for the interpolation of field values, which becomes problematic when examining bodies that are in direct proximity of each other or even colliding. To overcome this restriction, a detection of critical areas and a closure of the gap by an Immersed Boundary Method introducing an artificial wall boundary condition [5, 6] are embedded in the overset grid approach.
Exemplary applications are devoted to multiphase-flow conditions, offshore applications involving fluid-soil interaction and colliding cylinders.

[1] T. Rung, X. Luo and F. Matin. Multi-body Hydrodynamics using Parallel Overset-Grid Technique. In *ECCOMAS MARINE 2013*, Hamburg, Germany, 2013.

[2] S. Völkner and T. Rung. An Overset-Grid Three-Phase Flow Model for Offshore Operations. In *6th Int. Conference on Comp. Methods in Marine Engineering - MARINE 2015*, Rome, Italy, 2015.

[3] J. Brunswig and T. Rung. RANS Simulations Using Overset Meshes. In *4th Int. Conference on Comp. Methods in Marine Engineering - MARINE 2011*, Lissabon, Portugal, 2011.

[4] H. Hadzic. *Development and Application of Finite Volume Method for the Computation of Flows Around Moving Bodies on Unstructured, Overlapping Grids.* PhD Thesis, Hamburg University of Technology, 2005.

[5] R. Mittal and G. Iaccarino. Immersed Boundary Methods. In *Annu. Rev. Fluid Mech. 37*, 239-261, 2005

[6] R.W. Noack, D.A. Boger, R.F. Kunz and P.M. Carrica. Suggar++: An Improved General Overset Grid Assembly Capability. In *17th AIAA Computational Fluid Dynamics Conference* (AIAA 2009-3992), San Antonio, Texas, June 22-25, 2009.

Optimized simulation of multiscale problems on high-performance computers

M. Schlottke-Lakemper (RWTH Aachen University), H. Yu (RWTH Aachen University), S. Berger (RWTH Aachen University), M. Meinke (RWTH Aachen University), W. Schröder (RWTH Aachen University) 09:40

Noise emissions are a major concern in the transportation sector, especially in aviation. In Europe, the number of flights per year is projected to grow by 50% over the next 20 years. As a response, the European Commission has issued the goal to reduce the noise levels of flying aircraft by 65% until 2050. To achieve such optimizations, many aircraft components need to be analyzed in detail to understand their sound generation mechanisms and to subsequently improve their design. Therefore, highly parallelized numerical methods are required that allow to efficiently predict the flow field and the resultant far-field noise for realistic geometries. Due to the different spatial and temporal scales of the acoustic and hydrodynamic pressure fluctuations, however, a direct numerical simulation is often infeasible for applied problems. Thus, hybrid computational fluid dynamics (CFD) - computational aeroacoustics (CAA) schemes are the standard method for aeroacoustics simulations, where the flow solution and the acoustic pressure field are obtained with two independent solvers. Such an approach requires the exchange of information between the CFD and the CAA step, which is usually accomplished by storing acoustic source data on disk. This data exchange procedure represents a significant bottleneck for large-scale problems, however, as the parallel performance of the overall numerical method is limited by the bandwidth and scalability of the I/O subsystem.
In this contribution, we present a highly scalable direct-hybrid scheme that avoids these restrictions by executing the flow and the acoustics simulations simultaneously [1]. Both solvers operate on a joint hierarchical Cartesian mesh, which enables efficient parallelization [2] and inherently supports local grid refinement. A load-balanced domain decomposition is achieved by assigning different computational weights to the CFD and CAA cells, which are then distributed according to a space-filling curve. Since the joint mesh is partitioned such that corresponding flow and acoustics cells are allocated to the same subdomain, all data can be transferred directly in-memory. That is, no additional I/O or network operations are needed to exchange the source term information between the two simulations. The CFD solver is based on a finite-volume method and a discontinuous Galerkin scheme is used to solve the acoustic perturbation equations [3] for the noise propagation to the far field. To demonstrate the capabilities of the direct-hybrid approach, the aeroacoustic field of a pair of co-rotating vortices is determined. The results show that the direct-hybrid method can be used to efficiently obtain the acoustic pressure field and that it is suitable for highly parallel execution. In addition, when scaling to thousands of cores, the novel scheme exhibits superior performance in comparison to a classic hybrid solution with data exchange via disk I/O.

[1] M. Schlottke Lakemper, H. Yu, Sven Berger, M. Meinke, and W. Schröder. A fully coupled hybrid computational aeroacoustics method on hierarchical Cartesian meshes. *Comput. Fluids*, (accepted), 2016.

[2] A. Lintermann, S. Schlimpert, J. H. Grimmen, C. Günther, M. Meinke, and W. Schröder. Massively parallel grid generation on HPC systems. *Comput. Methods in Appl. Mech. Eng.*, 277:131–153, 2014.

[3] R. Ewert and W. Schröder. Acoustic perturbation equations based on flow decomposition via source filtering. *J. Comput. Phys.*, 188:365–398, 2003.

Building blocks for a leading edge high-order flow solver

I. Huismann (TU Dresden, Institut für Strömungsmechanik, Center for Advancing Electronics Dresden (cfaed)), J. Stiller (TU Dresden, Institut für Strömungsmechanik, Center for Advancing Electronics Dresden (cfaed)), J. Fröhlich (TU Dresden, Institut für Strömungsmechanik, Center for Advancing Electronics Dresden (cfaed)) 10:00

An important trend in Computational Fluid Dynamics is towards high-order methods, as they offer a substantially lower discretization error for the same number of degrees of freedom (DOF). Examples are the Spectral Element Methods (SEM) and Discontinuous Galerkin (DG) methods. Unfortunately, with most implementations the work load of such solvers increases drastically with the number of DOF, for example, when increasing the polynomial degree of the approximation. This issue gets particular pressing for elliptic solvers which are a vital building block in the time-stepping of the incompressible Navier-Stokes equations, resulting from pressure projection methods or implicit treatment of viscous terms. So far, this drastic increase of resources has hampered the use of SEM for higher polynomial degrees, such as 16 or more.

The present contribution is located at this particular "Frontier of CFD" and proposes an SEM with linear scaling in the number of degrees of freedom. It is achieved independent of the polynomial degree, independent of the aspect ratio of elements, and involves constant iteration count when increasing the number of elements. The method is based on combining static condensation with block-Jacobi preconditioning and iterative substructuring. The latter two lead to a constant iteration count, while the former warrants linear operator complexity.

In the presentation, the scheme is described in detail and applied to the construction of a Helmholtz solver. This solver is extremely fast and able to solve the Helmholtz equation with 10^{10} unknowns on 160 cores in acceptable time. It thus enables competitive high-order SEM simulations even on small clusters and in this way expands the frontier of CFD towards highly accurate results requiring comparatively modest resources.

Rotorcraft aeromechanics simulation

M. Keßler (Universität Stuttgart) 10:20

Helicopters in various configurations are probably the most complex aircraft in practical use today. Besides mechanical intricacies of their construction, aerodynamics contributes a significant share to this complexity. Nearly all well known flow phenomena do occur on rotorcraft, as laminar, transitional and turbulent flow at subsonic, transonic up to supersonic speeds, being highly instationary and three-dimensional, attached or separated, partly vortex dominated and overall highly interacting. In addition, the dynamics of the flexible rotor blades escalate the problem to a strongly fluid-structure coupled one, and the nonlinear and interlinked reaction to control angles like collective and cyclic pitch or attitude make the flight mechanics of helicopters notoriously difficult.

Simulation in general has helped the development of rotorcraft significantly, and Computational Fluid Dynamics especially has found its way into research as well as industrial application. Beyond sole performance estimates, highly detailed flow simulations can

reveal deep insights into flow physics and some interaction phenomena impossible to tackle with less sophisticated methods. Fluid-structure coupling at the rotor blades and free-flight trim to vanishing residual forces and moments, as necessary for stationary flight, have been proven indispensable to reach agreement to flight data. The geometric complexity of the rotor head including control rods and the swash plate can be of importance for some interaction phenomena. Recently, the inclusion of intake and exhaust flow as well as the consideration of flexibility at the tail boom has improved the level of sophistication further. High order discretisation schemes in conjunction with sufficient resolution in space and time allow simulation results of unprecedented quality, detail and reliability on high performance supercomputers with several ten thousand cores for real engineering questions. Of course, not all of those functionalities are to be applied for every simulation problem at hand, but the expected results have to be traded against (computational) cost. However, the tool chain has reached a level of maturity, where hard technical design decisions can be based dependably upon simulations as much as on wind tunnel experiments for various problems.

As is well known, rotorcraft are sources of significant sound emissions, depending on the model and the flight situation. As they often operate in or near residential areas, for example at hospitals, noise optimisation is of substantial importance for acceptance in society. Blade design optimisations as well as operational aspects can be beneficial, and CFD results with subsequent acoustic postprocessing are valuable in this regard as well. Of course, not only aerodynamic sources contribute to the overall noise, but engine, gearbox and others provide their dues either.

The presentation will give an overview of the techniques and functionalities developed at the helicopters & aeroacoustics group of the Institute of Aerodynamics and Gasdynamics over the last two decades. In addition to the current state of the art in rotorcraft simulation, ongoing projects and future trends within this area of application will be reported. Obviously, several key technologies are transferable to less demanding applications and thus valuable far beyond rotorcraft.

3 Young Researchers' Minisymposia

YR 1 : Computational Shape Optimization

Tuesday 09:00 - 11:00 Weimar hall, Seminar room 5

Organizers: Christian Kahle (TU München)
Martin Siebenborn (Trier University)

Shape optimisation with nonsmooth cost functions: from theory to numerics

K. Sturm (Johann Radon Institute for Computational and Applied Mathematics (RICAM)) 09:00

In this talk we consider a nonsmooth shape optimization problem. The cost function is of maximum-type and constrained by a quasi-linear partial differential equation in dimension two. We prove the Euler semi-differentiability and give a complete characterization of the derivative. We characterize stationary points and show how to compute steepest descent directions using kernel reproducing Hilbert spaces. Finally some numerical results are presented.

PDE-Constrained Shape Optimization with Fem-Tailored Discretization of Diffeomorphisms

P. Farrell, A. Paganini, F. Wechsung 09:20

PDE-constrained shape optimization problems are characterized by target functionals that depend both on the shape of a domain (the control) and on the solution of a boundary value problem formulated on that domain (the state).
There are conflicting demands on the discretization of the domain. On the one hand, k^{th}-order finite element approximation of the state suggests $W^{k,\infty}$-smooth domain deformations. On the other hand, typical isoparametric finite element discretization only allows $W^{1,\infty}$ piecewise polynomial representations of the domain geometry. How can the control and state spaces be discretized to satisfy these conflicting demands?
In this talk we develop a technique for cleanly decoupling a B-spline based *discretization of the control* and the *geometry used to solve the discretized state equation.* In particular, the discretized control satisfies the regularity requirement, which in turn guarantees that standard finite element estimates hold. As a consequence, the state can be approximated efficiently with typical finite element software.

Computational aspects of multigrid methods for optimization in shape spaces

V. Schulz, M. Siebenborn (Trier University), K. Welker (Trier University) 09:40

In many applications, which are modeled by partial differential equations, there is a small number of spatially distributed materials or parameters distinguished by interfaces. In order to identify these parameters, it is often more favorable to treat the shape of the interfaces as a variable instead of the parameter itself. Since the involved materials may form complex contours, high resolutions are required in the underlying finite element discretizations. The challenge here is to combine methods from PDE constraint shape optimization with HPC techniques and prepare algorithms for supercomputing.
We examine the interaction of multigrid methods and shape optimization in appropriate shape spaces. Our aim is a scalable algorithm for application on supercomputers, which can only be achieved by mesh-independent convergence. The impact of discrete approximations of geometrical quantities, like the mean curvature, on a multigrid shape optimization algorithm with quasi-Newton updates is investigated. For the purpose of illustration, we consider a complex model for the identification of cellular structures in biology with minimal compliance in terms of elasticity and diffusion equations.

[1] V. Schulz and M. Siebenborn: Computational comparison of surface metrics for PDE constrained shape optimization, Computational Methods in Applied Mathematics, 2016, (arXiv:1509.08601).

[2] M. Siebenborn and K. Welker: Computational aspects of multigrid methods for optimization in shape spaces, 2016, (arXiv:1611.05272).

Numerical aspects of unsteady fluid-structure interaction

J. Haubner, M. Ulbrich 10:00

In this talk we consider shape optimization for unsteady fluid-structure interaction problems that couple Navier-Stokes equations with non-linear elasticity equations. We focus on the monolithic approach in the Lagrangian framework. It is obtained by applying an ALE transformation to the fluid equations that are usually formulated on the time dependent physical domain. Shape optimization by the method of mappings approach requires another transformation which maps the ALE reference domain to a reference domain for shape optimization. This yields an optimal control setting and therefore can be used to drive an optimization algorithm with adjoint based gradient computation. Numerical results for our implementation, which builds on FEniCS, dolfin-adjoint, and IPOPT, are presented.

Drag Optimisation in a Stationary Navier-Stokes Flow Using a Phase Field Approach

K. Lam (University of Regensburg) 10:20

We present a phase field formulation for shape optimisation in stationary Navier-Stokes flow, with specific application to the study of drag minimisation, which has important consequences in the design of ships, race-cars, wind turbines and aircraft wings. With the help of a Ginzburg-Landau regularisation, we show that the resulting formulation

as an optimal control problem has at least one minimiser. Furthermore, first order necessary optimality conditions can also be derived, and together with a gradient flow approach, we use these conditions to numerically solve for the optimal shapes of drag minimisation.

YR 2 : Computational Techniques for Bayesian Inverse Problems

Tuesday 09:00 - 11:00 Weimar hall, Seminar room 2

Organizers: Björn Sprungk (TU Chemnitz)
Aretha Teckentrup (University of Edinburgh)

Well-posed Bayesian inverse problems and heavy-tailed stable quasi-Banach space priors

T. Sullivan (Freie Unviersität Berlin) 09:00

The framework of Bayesian inverse problems in infinite-dimensional parameter spaces, as advocated by Stuart (*Acta Numer.* 19:451–559, 2010) and others, is extended to the case of a heavy-tailed prior measure in the family of stable distributions, such as an infinite-dimensional Cauchy distribution, for which polynomial moments are infinite or undefined. It is shown that analogues of the Karhunen–Loève expansion for square-integrable random variables can be used to sample such measures on quasi-Banach spaces. Furthermore, under weaker regularity assumptions than those used to date, the Bayesian posterior measure is shown to depend Lipschitz continuously in the Hellinger and TV metrics upon perturbations of the misfit function and observed data.

A Transdimensional Bayesian Approach for Image Correction in Anisotropic Media

K. Tant (University of Strathclyde), A. Mulholland (University of Strathclyde), E. Galetti (University of Edinburgh), A. Curtis (University of Edinburgh) 09:20

The oil and gas, nuclear power and aerospace industries are just a subset of the sectors dependent on the routine maintenance of safety critical structures. Failure to detect structural weaknesses in components integral to the work being carried out by these industries can be catastrophic. Ultrasonic non-destructive testing is a technique which involves the transmitting of mechanical waves through the component under inspection. Just like in medical ultrasound, these waves can be passed through the component and subsequently collected without disturbing its internal composition. Large networks of sensors are deployed to carry out these inspections, resulting in massive quantities of noisy data, for which mathematical algorithms are required to decipher. Thus we are presented with an inverse problem: from this observed data, can we determine the path the ultrasound waves took and characterise any obstacles that they may have intercepted? Although there already exist techniques which can pick up on large scat-

tering events within the collected ultrasonic signals, small variances in the material microstructure can distort the image and lead to inaccurate characterisation and positioning of defects, particularly when the material is anisotropic or heterogeneous. This is why the development of an ultrasonic tomography system which can map out the material's internal structure is of industrial interest. Armed with this additional information, we can compensate for variances in the wave speed and improve our ability to correctly locate and characterise a defect. The work presented here endeavours to map the locally anisotropic grain structure typically exhibited in austenitic steel welds (which are notoriously difficult to inspect) using measured time-of-flight ultrasonic data. The reversible-jump Markov chain Monte Carlo method (RJMCMC) is an ensemble inference approach within a Bayesian framework. The material geometry is initially parameterised by a Voronoi tessellation, through which the wave path is modelled. The Voronoi diagram is then perturbed iteratively and the results are compared to the observed data using the Metropolis-Hastings criterion. If an iteration is accepted subject to this criterion, the respective Voronoi diagram contributes to the final ensemble solution. This final solution is a smooth map of the varying anisotropic regions of the sample. Using this map in conjunction with existing imaging algorithms, it is shown that an improvement in the overall flaw placement and characterisation can be achieved. Additionally, uncertainty maps can also be constructed where the variance of the value at each point in the spatial domain is plotted. These can be used to quantify the reliability of the extracted map.

Spectral nonlinear Kalman filtering

B. Rosic (TU Braunschweig), H. Matthies (TU Braunschweig) 09:40

Probabilistic parameter estimation of nonlinear systems is usually considered in a Bayesian framework in a sampling manner as analytical determination of posterior distributions is only possible in special cases when considered distributions are conjugate. In this talk an algebraic way of computing posterior estimates based on conditional expectation for any distribution type is presented. In this perspective special attention is paid to the design of a new nonlinear iterative filtering formula that has a Kalman-like flavour and is realised in a spectral functional representation form. The numerical procedures will be shown on some algebraic examples, as well as linear diffusion and nonlinear von Mises elastoplasticity problems.

Sequential Design of Computer Experiments for the Solution of Bayesian Inverse Problems

M. Sinsbeck (University of Stuttgart), W. Nowak 10:00

We present a sequential sampling method for the solution of Bayesian parameter inference problems. The model function is assumed to be computationally expensive, so the goal is to approximate the posterior with as few function evaluations as possible. To this end, the a priori unknown model function is described by a random field. The presented method classifies as a greedy one-step lookahead method: in each iteration, a

new point is selected such that the expected Bayes risk of the posterior distribution is minimized. Several numerical examples demonstrate that the expected Bayes risk is an appropriate refinement criterion for the solution of Bayesian inference problems. The presented approach shows to be more efficient than non-sequential sampling methods.

Uncertainty and constitutive model error quantification

I. Franck, P. Koutsourelakis 10:20

While for calibration purposes the solution of an inverse problem can almost always be achieved, underlying model inadequacies are barely considered. Traditional approaches use an additional regression model (e.g., Gaussian process) added to the model output [1], within a submodel [2] or reformulate the problem to a calibration problem (alone with regard to the model inadequacy [3]) to account for an underlying model error. This can either violate physical constraints, is infeasible in high dimensions or does not incorporated an inverse problem with regard to model parameters.
In this work we unfold conservation and constitutive laws to estimate model discrepancies and to simultaneously satisfy physical constraints. Efficient Bayesian strategies are incorporated when investigating in an inverse problem from solid mechanics. A correct identification of the mechanical properties of an unknown tissue and their corresponding uncertainties leads then to an accurate noninvasive, medical diagnosis.

[1] Kennedy, M. C. and O'Hagan, A. (2001), Bayesian calibration of computer models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 63: 425–464. doi:10.1111/1467-9868.00294

[2] Berliner, L. Mark., Jezek, K., Cressie, N., Kim, Y., Lam, C. and Van Der Veen, C. (2008). Modeling dynamic controls on ice streams: A Bayesian statistical approach. Journal of Glaciology, 54 (187), 705-714.

[3] Wu, Jin-Long, Jian-Xun Wang, and Heng Xiao. "A Bayesian Calibration–Prediction Method for Reducing Model-Form Uncertainties with Application in RANS Simulations." Flow, Turbulence and Combustion (2015): 1-26.

YR 3 : Local and Nonlocal Methods for Processing Manifolds and Point Cloud Data

Tuesday 09:00 - 11:00 Weimar hall, Wing hall

Organizers: Ronny Bergmann (TU Kaiserslautern)
Daniel Tenbrinck (WWU Münster)

Introduction

09:00

Interpolation on manifolds with B-splines

P. Gousenbourger (Université catholique de Louvain) 09:20

From a set of $n+1$ points p_i on a manifold $\mathcal{M}$ associated to nodes $i \in \mathbb{Z}$, we seek a $\mathcal{C}^1$ function : $\mathbb{R} \to \mathcal{M}$ such that $B(i) = p_i$.
To this end, we restrict B to a family of manifold-valued piecewise-Bézier curves where the first and last segments are quadratic while the others are cubic (as in [1]). We then compute the *control points* of B by generalizing the Euclidean concept of natural $\mathcal{C}^2$-splines.
One of the benefits of this application arise in problems whose solutions $(p_i)_{i=0}^n$ depend on only one parameter and are hard to compute, but are evaluated on a manifold $\mathcal{M}$. Hence, for a new value of the parameter, instead of solving the complicated problem, one can estimate the solution $p^\star$ by interpolating $(p_i)_{i=0}^n$ on $\mathcal{M}$.
The advantages of this technique are (i) a lower space complexity as the solution curve is represented by a few Bézier control points on the manifold, and (ii) a considerably simpler method that only requires two objects on the manifold: the Riemannian exponential and the Riemannian logarithm.

[1] P.-A. Absil, Pierre-Yves Gousenbourger, Paul Striewski, and Benedikt Wirth. Differentiable piecewise-B'ezier surfaces on Riemannian manifolds. SIAM Journal on Imaging Sciences, 9(4):1788–1828, 2016.

A Nonlocal Denoising Algorithm for Manifold-valued Images Using Second Order Statistics

J. Persch (Technische Universität Kaiserslautern) 09:40

Nonlocal patch-based methods, in particular the Bayes' approach of Lebrun, Buades and Morel [2013], are considered as state-of-the-art methods for denoising (color) images corrupted by white Gaussian noise of moderate variance. In this talk we present the first attempt to generalize this technique to manifold-valued images. Such images are frequently encountered in real-world applications, for example images with phase or directional entries appear in certain colormodels, or images with values in the manifold of symmetric positive definite matrices occur in diffusion tensor magnetic resonance imaging. We reinterpret the Bayesian approach of Lebrun et al. [2013] in terms of minimum mean squared error estimation, which motivates our definition of a corresponding estimator on the manifold. To do so we need to generalize the normal law to manifolds, which is not canonical. Different generalizations have already been proposed in the literature. Here we focus on an straightforward intrinsic model. With the estimator at hand we present a nonlocal patch-based method for the restoration of manifold-valued images. Various proof of concept examples demonstrate the potential of the proposed algorithm. This is joint work with Friederike Laus, Mila Nikolova, and Gabriele Steidl.

Retinal Image Analysis using Sub-Riemannian Geometry in SE(2)

E. Bekkers (Eindhoven University of Technology) 10:00

In our analysis of 2D Retinal images we represent the image data in higher-dimensional objects called orientation scores. Orientation scores are obtained via a wavelet-type transform with anisotropic filters. The resulting objects are densities on the (coupled) space of positions and orientations, which we identify with the roto-translation group SE(2). Due to the coupling of positions and orientations, and considering the fact that we analyze lifted (3D) representations of 2D data, we have to employ a sub-Riemannian geometry in our analyses. The sub-Riemannian geometry consists of the Lie group SE(2), a sub-bundle of the full tangent bundle which is defined via left-invariant vector fields, and sub-Riemannian metric tensor which measures the length of vectors in this sub-bundle. In this talk I will briefly give 3 examples of how we employ a sub-Riemannian geometry in retinal image analysis:

1. Vessel tracking: Curvature penalized vessel curves are found via the computation of sub-Riemannian geodesics in SE(2). Using orientation scores we first construct a data-adaptive sub-Riemannian metric; we then solve the sub-Riemannian eikonal equation, and obtain globally optimal geodesics via backtracking on the obtained sub-Riemannian distance maps.

2. Template matching: We find anatomical landmarks via cross-correlation based templates matching in orientation scores. The templates are learned via linear/logistic regression with a smoothing prior which we relate to Brownian motions SE(2).

3. Curvature biomarkers: We fit exponential curves in orientation scores which enables us to do pixel wise curvature measurements. These pixel wise measurements are used to compute global tortuosity measures which we show are significantly associated with hypertension and diabetes mellitus.

Robust Surface Reconstruction

V. Estellers (TUM) 10:20

We propose a method to reconstruct surfaces from oriented point clouds corrupted by errors arising from range imaging sensors. The core of this technique is the formulation of the problem as a convex minimization that reconstructs the indicator function of the surface's interior and substitutes the usual least-squares fidelity terms by Huber penalties to be robust to outliers, recover sharp corners, and avoid the shrinking bias of least-squares models. To achieve both flexibility and accuracy, we couple an implicit parametrization that reconstructs surfaces of unknown topology with adaptive discretizations that avoid the high memory and computational cost of volumetric representations. The hierarchic structure of the discretizations speeds minimization through multiresolution, while the proposed splitting algorithm minimizes non-differentiable functionals and is easy to parallelize. In experiments, our model improves reconstruction from synthetic and real data while the choice of discretization affects both the accuracy of the reconstruction and its computational cost.

4 DFG Priority Programmes

DFG-PP 1: Turbulent Superstructures

Organizer: Jörg Schumacher (TU Ilmenau, Fak. Maschinenbau)

DFG-PP 1 : Turbulent Superstructures

Tuesday 14:00 - 16:00 Coudraystr. 9A, Lecture hall 6

Turbulent Superstructures - An Introduction

J. Schumacher (TU Ilmenau, Fak. Maschinenbau) 14:00

The classical picture of turbulence which has prevailed since the pioneering works by Kolmogorov is that turbulent fluid motion is characterized by a cascade of vortices and swirls of different sizes that give rise to a featureless and stochastic fluid motion. Our daily experience shows, however, that turbulent flows in nature and technology are often organized in prominent large-scale and long-living structures that can cause extreme fluctuations. When present, superstructures dominate the global transport of mass, heat and momentum, they act as barriers to transport, and they increase the variability and fluctuations in the flow. Given the importance of superstructures for turbulent flows, we know very little about their origins, their dynamics, and their impact on turbulent flow properties. Furthermore, their consequences for the statistical properties of turbulent flows, and their connection to the occurrence of extreme events are poorly understood. The study of superstructures is now possible due to significant advances in measurement techniques, numerical simulation, and mathematical characterization. Tomographic laser-based measurement techniques can track the dynamics of turbulent structures with unprecedented resolution in space and time. Direct numerical simulations on massively parallel supercomputers have advanced to a level where turbulent flows in extended domains can be simulated at sufficiently high Reynolds numbers and in parameter ranges where superstructures emerge. Efficient methods to characterize dominant vortices and flow structures and to determine the transport across their boundaries as well as their dynamical evolution have been developed in applied mathematics. Computer science provides efficient algorithms for the visualization of structures in very large data sets. The presentation will give a compact overview on planned program activities.

Spectral Analysis of Large Scale Structures in Fully Developed Turbulent Pipe Flow

C. Egbers (BTU Cottbus - Senftenberg), A. Shahirpour (BTU Cottbus - Senftenberg), E. Öngüner (BTU Cottbus - Senftenberg), E. Zanoun (BTU Cottbus - Senftenberg) 14:20

Over the last decades, experimental and computational studies have resulted in considerable insight into physics of wall-bounded turbulent flows and have provided large turbulence data sets. Nevertheless, fundamental questions regarding structure and scaling of wall turbulence and coherent structures are still under debate. Therefore, the present work focuses on spectral analysis of experimentally measured data in Cottbus Large Pipe (CoLaPipe) test facility for a wide range of Reynolds numbers at low Mach numbers.

Spectral analysis of the velocity field can help to reveal insightful information about the behavior of structures with different wavelengths. The pre-multiplied velocity spectrum that represents the energy distribution in the wave number space helps to follow the foot prints of such structures and provides an estimate of their energy content. At sufficiently high Reynolds numbers and at certain wall-normal locations, two peaks are observable in the outer region of the pre-multiplied spectra, which can be interpreted as signatures of Large Scale Motions (LSM) and Very Large Scale Motions (VLSM) (see, e.g., Rosenberg et al. 2013, Vallikivi et al. 2015).

In the same manner, the present study aims at describing the most energetic motions found in experimental data measured in CoLaPipe, in terms of their wave lengths, wall-normal locations and energy content and their scaling. Experiments are conducted, utilizing the CoLaPipe at bulk Reynolds numbers of $6 \times 10^4 < Re_b < 10 \times 10^6$, where Re_b is based on the pipe diameter D and bulk velocity U_b, at Mach numbers $Ma < 0.23$. Measurements have been carried out using Hot Wire Anemometry (HWA) and Particle Image Velocimetry (PIV).

Acknowledgments: This project is funded inside the DFG-SPP (1881) "Turbulence and Superstructures" under grant no. EG100/24-1.

Turbulent Superstructures in Controlled Flows

D. Gatti, A. Stroh, Y. Hasegawa, B. Frohnapfel 14:40

The term "turbulent superstructure" (TSS) is used to describe certain patterns observed in wall-bounded shear flows at very high Reynolds numbers. These patterns, e.g. connected regions of relatively low speed fluid, are typically very elongated in streamwise direction. They are often described through the premultiplied streamwise velocity spectra in which a second peak emerges at high Reynolds numbers. Since TSS are known to carry a large amount of the Reynolds shear stress - which represents the turbulent contribution to skin friction drag - it is speculated whether or not the potential control of such structures could lead to significant drag reduction. The present contribution aims at improving our understanding of the link between TSS and skin friction drag through a numerical experiment. DNS of a turbulent channel flow is carried out at Re_-

tau=1000. While this friction Reynolds number is fixed through a prescribed pressure gradient the turbulent flow is modified with different near-wall control techniques. In the present setting with a fixed friction Reynolds number these control techniques lead to an increased flow rate. We investigate how these changes reflect in the spectral representation of the streamwise velocity fluctuations (and hence TSS) and most importantly in the corresponding spectral representation of the Reynolds shear stress.

Trajectory-based computational study of coherent behavior in flows

K. Padberg-Gehle (Leuphana Universität Lüneburg) 15:00

The notion of coherence in time-dependent dynamical systems is used to describe mobile sets that do not freely mix with the surrounding regions in phase space. In particular, coherent behavior has an impact on transport and mixing processes in fluid flows. The mathematical definition and numerical study of coherent structures in flows has received considerable scientific interest for about two decades, see [1] for a recent review and comparison of different approaches. However, mathematically sound methodologies such as transfer-operator-based schemes [2] require full knowledge of the flow field or at least high resolution trajectory data, which may not be available in applications.
Recently, different computational methods have been proposed to identify coherent behavior in flows directly from Lagrangian trajectory data, such as obtained from particle tracking algorithms. In this context, spatio-temporal clustering algorithms have been proven to be very effective for the extraction of coherent sets from sparse and possibly incomplete trajectory data [3, 4, 5].
Inspired by these recent approaches, we consider an unweighted, undirected network with Lagrangian particle trajectories serving as network nodes. A link is established between two nodes if the respective trajectories come close to each other at least once in the course of time. Classical graph algorithms are then employed to analyze the resulting network. In particular, spectral graph partitioning schemes allow us to identify coherent sets of the underlying flow. The proposed method is very fast to run and we demonstrate its applicability in a number of example systems. Furthermore, we point out theoretical links to other approaches.

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[2] Froyland, G. and Padberg-Gehle, K.: Almost-invariant and finite-time coherent sets: directionality, duration, and diffusion, in: Bahsoun, W., Bose, C., and Froyland, G. (eds.): Ergodic Theory, Open Dynamics, and Coherent Structures, vol. 70 of *Proceedings in Mathematics and Statistics*, pp. 171–216, Springer, 2014.

[3] Froyland, G. and Padberg-Gehle, K.: A rough-and-ready cluster-based approach for extracting finite-time coherent sets from sparse and incomplete trajectory data, Chaos, 25, 087406, 2015.

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[5] Banisch, R. and Koltai, P.: Understanding the geometry of transport: diffusion maps for Lagrangian trajectory data unravel coherent sets, https://arxiv.org/abs/1603.04709, 2016.

Symmetry induced new non-modal eigenfunctions in hydrodynamic stability theory and non-exponential growth rates

M. Oberlack (TU Darmstadt) 15:20

Classical hydrodynamic stability theory for laminar shear flows, no matter if considering long-term stability or transient growth, is based on the normal-mode ansatz, or, in other words, on an exponential function in space (stream-wise direction) and time. Recently, it became clear that the normal mode ansatz and the resulting Orr-Sommerfeld equation is based on essentially three fundamental symmetries of the linearized Euler and Navier-Stokes equations: translation in space and time and scaling of the dependent variable - independent of the base flow, which is analyzed on its stability. Further, Kelvin-mode of linear shear flows seemed to be an exception in this context as it admits a fourth symmetry resulting in the classical Kelvin mode which is rather different from normal-mode. However, very recently it was discovered that most of the classical canonical shear flows such as linear shear, Couette, plane and round Poiseuille, Taylor-Couette, Lamb-Ossen vortex or asymptotic suction boundary layer admit more symmetries. This, in turn, led to new problem specific non-modal ansatz functions. In contrast to the exponential growth rate in time of the modal-ansatz, the new non-modal ansatz functions usually lead to an algebraic growth or decay rate, while for the asymptotic suction boundary layer a double-exponential growth or decay is observed. Some of the new non-modal eigenvalue problems have been solve analytically and first results will be presented.

Turbulent superstructures in thermal convection flows

A. Pandey (TU Ilmenau), J. Schumacher (TU Ilmenau) 15:40

When turbulent convection proceeds in horizontally extended layers large-scale patterns of the time-averaged velocity and temperature fields are formed. These patterns are termed turbulent superstructures and are studied here by means of three-dimensional direct numerical simulations in closed rectangular cells with an aspect ratio of 25:25:1. A spectral element method is applied which uses Lagrangian interpolation polynomials on the basis of Legendre functions for the spectral expansion of the turbulent fields on each element. We present a series of simulations at three Prandtl numbers and different Rayleigh numbers. The Prandtl numbers are Pr=7 for convection in water, Pr=0.7 for convection in air and Pr=0.021 for convection in a liquid metal such as mercury. Rayleigh numbers are chosen with values even and larger than Ra=1e5. The investigation of instantaneous and time-averaged velocity and temperature patterns is reported as well as a statistical analysis of the typical spatial correlation scales and fluctuations. Furthermore, it is reported how the global transport of heat and momentum across the fluid layer compares with previous simulations in other geometric configurations. This

work is supported by the Priority Programme SPP 1881 of the Deutsche Forschungsgemeinschaft.

DFG-PP 2: Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis

Organizer: Jörg Schröder (Universität Duisburg-Essen)

DFG-PP 2 : Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis

Tuesday 16:30 - 18:30 Coudraystr. 9A, Lecture hall 6

SPP1748 - Reliable Simulation Techniques in Solid Mechanics. Development of Non-standard Discretization Methods, Mechanical and Mathematical Analysis.

J. Schröder (Universität Duisburg-Essen), C. Carstensen (Humboldt-Universität zu Berlin) 16:30

This talk gives an overview on the German priority programme 1748 (DFG SPP 1748). Numerical simulation techniques are an essential component for the construction, design and optimisation of cutting-edge technologies as for example innovative products, new materials as well as medical-technical applications and production processes. These important developments pose great demands on quality, reliability and capability of numerical methods, which are used for the simulation of these complex problems. Challenges are for example capture of incompressibility, anisotropy and discontinuities. Existing computer-based solution methods often provide approximations which cannot guarantee substantial, absolutely necessary stability criteria respectively fulfill them. Especially in the field of geometrical and material non-linearity such uncertainties appear. Typical problems are insufficient or even pathological stress approximations due to unsuitable approximation spaces as well as weak convergence behaviour because of stiffening effects or mesh distortion. Similar problems arise in the framework of crack and contact problems. Here the resolution of the local discontinuities as well as their evolution plays a key role. The scientists of the SPP 1748 have set themselves the goal to establish a new quality in the area of non-conventional discretisation methods. Herein the work programme of the SPP is founded: The evolution of modern non-conventional discretisation methods, their mathematical analysis and the exploration of their application limits on the basis of suitable benchmark problems.

The following projects are currently part of SPP 1748:

- Adaptive isogeometric modeling of propagating strong discontinuities in heterogeneous materials
- Finite element approximation of functions of bounded variation and application to models of damage, fracture and plasticity
- Foundation and application of generalized mixed FEM towards nonlinear problems in solid mechanics
- High-order immersed-boundary methods in solid mechanics for structures generated by additive processes
- Hybrid discontinuous Galerkin methods in solid mechanics
- Isogeometric and stochastic collocation methods for nonlinear probabilistic multiscale problems in solid mechanics
- First-order system least squares finite elements for finite elasto-plasticity
- Advanced Finite Element Modelling of 3D Crack Propagation by a Phase Field Approach
- Novel finite elements for anisotropic media at finite strain
- Large-scale simulation of pneumatic and hydraulic fracture with a phase-field approach
- A novel smooth discretization approach for elasto-plastic contact of bulky and thin structures

A fictitious domain method for problems of structural mechanics

A. Düster (Technische Universität Hamburg), S. Kollmannsberger (Technische Universität München), E. Rank (Technische Universität München), A. Schröder (Paris Lodron Universität Salzburg) 16:50

The finite cell method (FCM) is a combination of the fictitious domain approach with high-order finite elements. Thanks to the use of Cartesian grids, the pre-processing, i.e. mesh generation is significantly simplified. However, due to the fact that the applied meshes do not conform to the geometry of the problem, special care has to be taken with respect to the numerical integration of the weak form, the local refinement of the approximation as well as the treatment of boundary conditions.

The FCM has been applied to several problems like linear elasticity as well as to problems in biomechanics or wave propagation. Nonlinear problems such as geometrical nonlinearities or elastoplasticity have been addressed, too. The FCM has also been successfully applied to the numerical homogenization of materials with complicated microstructure or to topology optimization in structural mechanics.

The talk is intended to give an overview over the finite cell method and its applications to solid mechanics. Special emphasis will be placed on improved quadrature schemes to accelerate the numerical integration of cell matrices. Furthermore, local enrichment based on the partition of unity method and the multi-level *hp*-refinement will be discussed. The applications to be presented will range from linear elastostatic analysis to problems of large deformations. We will also present some first results related to the simulation of additive manufacturing by means of selective laser melting where the FCM is applied to solve the transient thermo-mechanical problem with phase changes.

[1] A. Düster, E. Rank, B. Szabó. The p-Version of the Finite Element and Finite Cell Methods. In E. Stein, R. de Borst, T.J.R. Hughes, editors: Encyclopedia of Computational Mechanics. Volume 2: Solids and Structures, John Wiley & Sons, 2017.

[2] M. Joulaian, S. Hubrich, A. Düster. Numerical integration of discontinuities on arbitrary domains based on moment fitting. Computational Mechanics, 57:979-999, 2016.

[3] L. Kudela, N. Zander, S. Kollmannsberger, E. Rank. Smart octrees: Accurately integrating discontinuous functions in 3D. Computer Methods in Applied Mechanics and Engineering, 306:406-426, 2016.

Pitfalls and Remedies in the Approximation of Stresses for Linear and Nonlinear Elasticity

G. Starke (Universität Duisburg-Essen), F. Bertrand (University of Duisburg-Essen) 17:10

This presentation is concerned with the accuracy of stresses computed from displacement and, possibly, pressure approximations associated with finite element methods. It is shown that local stress components are rather poorly represented by some finite element approaches and an explanation for this will be given. These issues become particularly apparent if surface traction forces are evaluated. On the other hand, these problems disappear if nonconforming finite element approaches are used which will also be explained. The relation to stress-reconstruction techniques for linear elasticity in two and three space dimensions will be discussed. Finally, the difficulties with extending these techniques to nonlinear elasticity and to curved boundaries are discussed.

A Virtual Element Method for Large Deformation Contact

W. Rust (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), B. Reddy (University of Cape Town), B. Hudobivnik (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 17:30

When dealing with contact problems a wide range of methods is available. In the finite element environment Lagrange multipliers or penalty methods are widely used to enforce constraints. In the development of contact procedures the main focus, next to accuracy, is laid on the robustness of the method. However, improvements like the enhancement of the surface interpolation or the constraint discretization also increase the complexity of the implementa- tion. One of the easiest treatments is the nodalwise enforcement of the contact constraints. This requires pairs of nodes in the contact zone that are not necessarily given for general meshes.

In this context the method of the virtual element method [1] offers a more flexibel discretization allowing for a node insertion algorithm creating nodal pairs for non-matching interfaces [2]. By using „virtual“ polynomial basis functions an arbitrary number of nodes per element with an arbitrary elementgeometry can be represented. Starting with a quick overview over the basic method of these virtual functions, the talk will then discuss the changes made for the formulation of the method for higher order basis functions and large deformations.

When aproximating elements with different node numbers using the same basis function, an error occurs that can be summarized in an error term. In the small deformational setup this extra error term can be computed and is then used to stabilize the method. However during the derivation of the large deformational case several assumptions regarding the computation of the error term have to be made that lead to bad convergence behaviour. This setback is overcome by the use of automatic differentiation guaranteeing an accurate solution.

After showing the behaviour of these polygonal elements for large deformations, the virtual elements are then applied to the contact procedure. In the examples it is demonstrated how the node insertion and deletion algorithm makes it possible to use the node-to-node contact formulation in a large deformational setup.

[1] Beirão da Veiga L., Brezzi F., Cangiani A., Manzini G., Marini L.D., Russo A. Basic principles of virtual element methods. *Mathematical Models and Methods in Applied Sciences.* 23(01), 199-214 (2013).

[2] Wriggers P., Rust W.T., Reddy B.D. A virtual element method for contact. *Computational Mechanics.* 58(06), 1039–1050, Springer Berlin Heidelberg (2016)

Quasi-optimal Adaptive Mesh Refinement and Superior Eigenvalue Approximation in Isogeometric Analysis

P. Hennig (TU Dresden), M. Kästner (TU Dresden), P. Morgenstern (Universität Bonn), D. Peterseim (Universität Bonn) 17:50

This talk presents novel adaptive mesh refinement procedures for T-splines and hierarchical B-splines in the context of computational partial differential equations. The

procedures are provably quasi-optimal and, hence, adaptive spline-based discretizations may achieve optimal convergence rates for linear elliptic model problems. The new approaches are studied numerically and compared with previous ones in a series of benchmark problems.
In addition, the talk discusses global stability properties of the Rayleigh-Ritz approximation of eigenvalues of the Laplace operator by B-splines and the possible superiority of smooth splines over classical finite elements in this regard.

Discontinuous Galerkin method in 3D linear elastic problems with application in problems with locking

H. Bayat (RWTH Aachen University), S. Kastian, S. Wulfinghoff (Institute of Applied Mechanics, RWTH Aachen University), S. Reese (Institute of Applied Mechanics, RWTH Aachen University) 18:10

In the present work, a three-dimensional discontinuous Galerkin (DG) formulation is presented and investigated for linear elastic problems. Among different variations of DG methods, the incomplete interior penalty Galerkin IIPG method is applied here, where the symmetry term is absent and the approach is stable through the application of a penalty term.
Due to the discontinuity of the DG elements, a new meshing approach is introduced and applied in the finite element analysis program FEAP. This results in a shorter calculation time due to the improved band width of the stiffness matrix. Additionally, different examples are calculated to investigate the locking behavior of the DG method compared to CG method. A locking-free 3D element Q1SP is applied to investigate and compare the locking behavior. Moreover, the combination of the latter element with DG element is examined to observe if the locking problem can be further avoided.

DFG-PP 4: Field Controlled Particle Matrix Interactions: Synthesis Multiscale Modeling and Application of Magnetic Hybrid Materials

Organizer: Stefan Odenbach (TU Dresden)

DFG-PP 4 : Field Controlled Particle Matrix Interactions: Synthesis Multiscale Modeling and Application of Magnetic Hybrid Materials

Tuesday 14:00 - 16:00 Coudraystr. 11C, Room 101

Microstructure analysis in magnetorheological elastomers – and other magnetic particle based materials

S. Odenbach (TU Dresden) 14:00

The knowledge of changes in the micro-structure of magnetorheological materials, i.e. a knowledge concerning the spatial arrangement of the magnetic particles and its changes due to external stimuli is an important prerequisite for a detailed understanding of the magnetic field driven effects found in these materials. Detailed microstructural data can serve as well as input for simulations of the behavior of magnetorheological materials as it can provide a benchmark for theoretical results. Using X-ray microtomography (X-µCT), it becomes possible to produce three dimensional representations of macroscopic samples of magnetorheological materials with a spatial resolution allowing for single particle identification. By means of digital image processing these data sets can be evaluated in detail, providing information about changes driven by different production parameters of magnetorheological elastomers [1, 2] or the influence of external stimuli on macro- and microstructure [3]. Moreover not only normal magnetorheological elastomers can be investigated, but also more complex structures like magnetorheological foams [4], where the micro-structure of the matrix can be determined together with the particle arrangement, and even liquid magnetorheological materials can be subject to microstructural investigations using X-µCT [5]. The presentation will outline the techniques needed for such investigations as well as the experimental possibilities arising here and will embed them into the framework of SPP1681.

Acknowledgments Financial support by DFG under grant No. OD18/21 within SPP1681 is gratefully acknowledged.

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[2] T. Borbáth, S. Günther, D. Yu. Borin, Th. Gundermann, S. Odenbach. (2012) Smart Mater. Struct. 21 105018

[3] Th. Gundermann, S. Günther, D. Borin, S. Odenbach (2013) J. Phys.: Conf. Ser. 412 012027

[4] M. Schümann, S. Günther, S. Odenbach (2014) Smart Mater. Struct. 23 075011
[5] T. Borbáth, I. Borbáth, S. Günther, O. Marinica, L. Vékás, S. Odenbach (2014) Smart Mater. Struct. 23 055018

Buckling of paramagnetic chains in soft gels

S. Huang (Max-Planck-Institut für Polymerforschung Mainz), G. Pessot, P. Cremer, R. Weeber, C. Holm, J. Nowak, S. Odenbach (Lehrstuhl für Magnetofluiddynamik, Mess- und Automatisierungstechnik, TU Dresden), A. Menzel (Institute of Mechanics, TU Dortmund and Division of Solid Mechanics, Lund University), G. Auernhammer (Max-Planck-Institut für Polymerforschung) 14:20

We study the magneto-elastic coupling behavior of paramagnetic chains in soft polymer gels exposed to external magnetic fields. To this end, a laser scanning confocal microscope is used to observe the morphology of the paramagnetic chains together with the deformation field of the surrounding gel network. The paramagnetic chains in soft polymer gels show rich morphological shape changes under oblique magnetic fields, in particular a pronounced buckling deformation. The details of the resulting morphological shapes depend on the length of the chain, the strength of the external magnetic field, and the modulus of the gel. Based on the observation that the magnetic chains are strongly coupled to the surrounding polymer network, a simplified model is developed to describe their buckling behavior. A coarse-grained molecular dynamics simulation model featuring an increased matrix stiffness on the surfaces of the particles leads to morphologies in agreement with the experimentally observed buckling effects.
Huang, S. et al., Soft Matter (2016), 12, 228.

Modeling of magnetic hystereses in soft MREs

K. Kalina (TU Dresden), J. Brummund (TU Dresden), P. Metsch (TU Dresden), M. Kästner (TU Dresden) 14:40

Magnetorheological elastomers (MREs) are a class of composites which can alter their macroscopic properties if a magnetic field is applied. These materials consist of a polymer matrix with embedded micron-sized magnetizable particles. If the magnetic filler consists of magnetically soft particles as carbonyl iron, the rearrangement of the microstructure due to the external magnetic field is reversible, whereas MREs which contain magnetically hard particles as NdFeB reveal irreversible microstructural alterations. Experiments published by Linke et al. [1] indicate that the hystereses are significantly smaller if the NdFeB particles are embedded into a soft polymer instead of a comparably stiff epoxy matrix.
To investigate the microstructural causes of the measured macroscopic hysteresis, a microscale model based on a general continuum formulation is presented in this contribution. The magnetic behavior of the embedded NdFeB-particles is described by a rate independent vector hysteresis model which is based on the work of Bergqvist [2]. The governing equations of the coupled magnetomechanical problem are solved within a nonlinear finite element formulation as used in [3]. In order to connect the macroscopic and

the microscopic magnetic and mechanical quantities, a suitable homogenization scheme is applied.
Simulations presented in this contribution indicate a rotation of the particles within the soft polymer material. Due to this effect, the effective hystereses of the MRE are significantly smaller than the hystereses of pure NdFeB. The presented computational results are qualitatively in good agreement with the results in [1].
Acknowledgements:
The present study is funded by the German Research Foundation (DFG), Priority Program (SPP) 1681, grant KA 3309/2-2.

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Modeling and Numerical Simulation of Ferrogels Containing Mobile Magnetic Particles

A. Attaran (TU Dresden, Institut für Festkörpermechanik), T. Wallmersperger (TU Dresden, Institut für Festkörpermechanik) 15:00

Ferrogels are multicomponent materials consisting of a chemically cross-linked polymer network, fixed and mobile magnetic nanoparticles as well as a liquid. Based on their multicomponent nature, a continuum model for ferrogels was developed by the authors [1]. In that modeling approach, the field equations of ferrogels were derived within the framework of the theory of mixtures. By introducing a suitable free energy function, thermodynamically consistent constitutive laws were presented.
For the purpose of numerical simulation, however, the model as mentioned above was simplified to contain fixed magnetic particles and the polymer network only. By using this model, a magneto-mechanical formulation was obtained. The reduced model was numerically treated using the finite element method to investigate the deformation of ferrogels in a magnetic field. An elongation of a ferrogel was observed parallel to the applied magnetic field.
Towards extending the simplified model for ferrogels, mobile magnetic particles are considered in the present work additionally. By including them, diffusion of mobile magnetic particles inside the gel, in the absence and in the presence of an externally applied magnetic field, is studied. In the course of diffusion, parts of the mobile particles can be converted into fixed magnetic particles or become trapped within the polymer network.

[1] A. Attaran, J. Brummund, and T. Wallmersperger, “Development of a continuum model for ferrogels,” *Journal of Intelligent Material Systems and Structures*, p. 1045389X16672564, 2016.

Magnetic Nanocubes in Self-Assembled Hydrogels

S. Schatte (Technische Universität Berlin - Institut für Chemie), M. Gradzielski (Technische Universität Berlin - Institut für Chemie), S. Prévost (ESRF - The European Synchrotron) 15:20

Thermoresponsive aqueous ferrogels with cubic magnetic nanoparticles (MNPs) incorporated into a self-assembled network are studied primarily by small angle scattering (SAS), rheology and electron microscopy. Comprehension of the interplay between network and MNPs enables manipulation of responses to mechanical stress, temperature and magnetic field. Most ferrogels result from the addition of polymeric gelators to an existing ferrofluid.[1] The resulting ferrogels are composed of pockets of the original ferrofluid encapsulated by domains of polymer molecules at colloidal scale. Thus, such systems do not exhibit any significant synergistic response. A more elaborated ferrofluid, which can respond to stimuli, is thereby constructed by incorporation of monodisperse silica coated MNPs into a gel network, which interacts with them. Small angle scattering (SANS, SAXS) is used to get a detailed picture of particle and gel fiber arrangement at nanoscale, while time-resolved SAS shows the kinetics of such systems (relaxation time and pathway of particles and network). A new class of gels discovered within this project is based on combining fatty acids with basic amino acids. Such gels are eco-friendly, non-toxic, cheap and present attractive rheological and temperature-dependent properties. The viscosity changes reversibly over orders of magnitude by heating/cooling. By pH-variation, the system switches from a vesicle gel to a viscoelastic network formed by worm-like micelles, which is a very elegant way of tuning structure and properties. Highly monodisperse Fe3O4, CoFe2O4 (hard ferrite), MnxZn1-xFe2O4 (soft ferrite) nanocubes in a size range of 7 to 17 nm (edge length, corresponding to 10 to 30 nm space diagonal) were synthesized using a thermal decomposition route[2] resulting in a large scale reaction (2-3 gram). Such monodisperse nanoparticles are required for detailed structural investigations (SAS). Commercial ferrofluids are not suitable due to high polydispersity. In order to enhance colloidal stability and integrate these hydrophobic magnetic nanoparticles into a hydrogel network, they need to be surrounded by a protective shell, which subsequently can be modified chemically. A silica coating[3] has been obtained via reverse -emulsion reactions. The particles are water dispersible with a homogeneous shell, whose thickness is tunable between 4 and 15 nm. The aim is to combine MNPs and gels to self-assembled ferrogels, whose properties cannot only be controlled by pH, temperature and composition, but also by a possible hydrophobic modification of the silica shell resulting in a versatile system of a responsive ferrogel.

This work is supported by DFG PR1473/1 within the Priority Program SPP1681.

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DFG-PP 4 : Field Controlled Particle Matrix Interactions: Synthesis Multiscale Modeling and Application of Magnetic Hybrid Materials

Tuesday 16:30 - 18:30 Coudraystr. 11C, Room 101

Magnetomechanical properties of magnetic hybrid elastomers

D. Borin (TU Dresden), G. Stepanov (State Research Center GNIICHTEOS), S. Odenbach (TU Dresden) 16:30

The solid analogous of magnetorheological (MR) fluids are elastomers, in which the liquid carrier medium is replaced by a rubber or gel-like matrix (MREs) [1,2]. The most prominent property of these controllable elastomers is the MR effect. In the context of the elastomer it is an increase of elasticity in an external magnetic field. Physical properties of MREs are strongly correlated with their microstructure. Being once cured, conventional MREs based on carbonyl iron powder have certain properties which are controllable with an applied field. However, these characteristics can only be tuned by means of this external stimulus. Recently the use of a magnetically hard component, which enables the adjustment of the elasticity of MREs after they are cured, has been proposed [3]. In this contribution we report on the influence of the powder composition on the magnetomechanical response of MREs. Our study is focused on a comparison of the samples of MRE with different elasticity filled with a soft magnetic powder as reference samples and samples based on hard magnetic powder and complex mixtures of both types of powder. MREs with the complex powder are called magnetic hybrid elastomers. Samples with the hybrid composition as well as specimens containing the magnetic hard component only were magnetized prior to the testing procedure in order to obtain a remanence magnetization. Experimental characterization of the samples has been performed using various types of instrumentation, including oscillating rheometry, axial quasi-static and dynamic loading and others.

Acknowledgements:

Financial support by Deutsche Forschungsgemeinschaft (DFG) under Grant Bo 3343/1-1 within PAK 907 providing the basis for our investigations is gratefully acknowledged. G.S. would like to acknowledge the support of RFBR under Grant 16-53-12009.

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Magnetically induced movement of NdFeB particles in magnetorheological elastomers

M. Schümann (TU Dresden/ Institut für Stroemungsmechanik), R. Müller, S. Odenbach (TU Dresden/ Institut für Stroemungsmechanik) 16:50

Introduction

Magnetorheological elastomers are a special kind of magnetic field-responsive smart materials devel-oped in the last years, where magnetic micro particles are embedded in a soft elastomer matrix. As a result the magnetoactive effects on the mechanical properties are combined with a soft elastic mate-rial. The investigation of the interaction of the particles with the external magnetic fields and the matrix is a subject of ongoing research. X-ray micro tomography proved to be a convenient tool for analysis of the particle micro structure [1, 2]. For this investigation a stepwise magnetisation of the material up to 2 T was performed to retrace the chain formation process of the particles. A broad analysis of the change of the magnetic, mechanical and structural properties should provide an un-derstanding in the chain formation process.

Material and methods

40 wt% of Magnequench MQA were used as magnetic NdFeB particles. These are highly anisotropi-cally shaped. By sieving the particles a size range of 100 to 200 µm was obtained. Gelest DMS-V25 prepolymer and HMS-151 cross- linker were used to produce a soft elastomer ma-trix. The utilization of this material enables the precise adjustment of the elastic modulus and reac-tion time (by the variation of the amount of added catalyst). The polymerized samples were tested with a DYNA-MESS universal testing machine with and without the presence of an external magnetic field with a flux density of 240 mT. Subsequently, the sample was tomographed with the TomoTU cone beam tomography setup with and without the presence of a 240 mT field as well. The samples were than magnetised at 250 up to 2.000 mT in 250 mT steps. After each magnetisation the measurements were repeated. Additionally the material was analysed by XRD to explain the orientation behaviour of the particles as well with VSM to measure the remaining magnetisation after each step.

Magnetorheological effect

The results regarding the elastic properties show a signifcant increase of the Young's modulus above a magnetisation of 1 T, both in presence of the 240 mT field and without. This leads to a significant magnetorheological effect above 1 T as well. A slight decrease of the modulus without the field is prominent. This can be explained with the fatigue of the sample due to the local destruction of the matrix as a result of the advancing particle displacement.

Particle structure

The reconstructed tomography data shows the stepwise rearrangement of the particles form a homo-geneous distribution to fully formed chains. This changing structure leads to the elastic properties observed with the mechanical testing. It's worth noticing, that the particles align perpendicular to the direction of the magnetic field. This occurs not just with tightly packed chains but also with weak fields and only a slight rotation of the particles. X-ray Diffraction measurements (XRD) show a clear relation between geometrical orienta-tion and crystal orientation of the particles. Thus it can be assumed, that the particles align their magnetic predominant direction of the crystal structure to the magnetic field. The fact that the magnetic predominant direction of the particles is perpendicular to their longest axis can be linked to a preferred fractioning direction of the crystals during the particle manufacturing. Particle tracking

Digital image processing and segmentation allows an evaluation of geometric data ob-

tained by to-mography (position, size, surface and main axes) of every single particle [3]. A particle-particle as-signment was already conducted for the initial state. This allows to track the translation and rotation of every specific particle and will be expanded to track single particles from their initial state to the state of fully formed chains.

Acknowledgments
Financial support by DFG (Grant. No. OD18/21) within SPP1681 is gratefully acknowledged.

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Force- and torque-induced matrix-mediated interactions between rigid inclusions in elastic media

M. Puljiz (Heinrich-Heine-Universität Düsseldorf), S. Huang 17:10
(Max-Planck-Institut für Polymerforschung Mainz), G. Auernhammer
(Max-Planck-Institut für Polymerforschung Mainz), A. Menzel
(Heinrich-Heine-Universität Düsseldorf)

We consider rigid spherical particles embedded in a soft elastic matrix. The matrix sticks to the surfaces of the particles. Then we impose forces and/or torques on these particles. In principle any additional force and/or torque can be considered, while here we concentrate on magnetic forces induced between the particles by an external magnetic field.

Through the forces and torques, the particles get displaced and rotated against the surrounding matrix. This leads to matrix deformations and consequently to counteractions. The resulting deformation fields in the matrix are long-ranged. Particularly, they influence other embedded rigid particles and lead to additional displacements and rotations. Moreover, since the particles are rigid, they resist deformations. In turn, this likewise affects the matrix deformations, which further modifies the resulting particle displacements and rotations.

Overall, the displacements and rotations of the particles are highly coupled due to their interactions via the embedding elastic matrix. Addressing the problem by direct numerical simulation is of a certain computational effort, as the deformation of the matrix must be explicitly resolved. However, we could recently derive explicit analytical expressions for the coupled displacements and rotations as a function of *only* the imposed forces and torques as well as the particle coordinates [1, 2]. The role of the embedding elastic matrix is implicitly included in these expressions and does *not* need to be explicitly resolved any more. We have tested and verified our theory by comparison with experiments [1]. There, magnetic interactions between embedded paramagnetic particles were induced by external magnetic fields. Theory and experiments show very good agreement.

To perform our derivation, we have adapted an iterative procedure from low-Reynolds-number hydrodynamics [3, 4]. In hydrodynamics, the method was highly successful

in describing the behavior of fluid colloidal suspensions. Considering the importance of the method in hydrodynamics, we expect similar relevance of our approach in the characterization of tunable elastic composite materials in the future.

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Nanorheology - Dynamics of magnetic nanoparticles in non-Newtonian media

H. Remmer (TU Braunschweig), E. Roeben (Universität zu Köln), K. Birster (Universität des Saarlandes), A. Tschöpe (Universität des Saarlandes), A. Schmidt (Universität zu Köln), F. Ludwig (TU Braunschweig) 17:30

Whereas the Brownian relaxation of magnetic nanoparticles (MNP) in Newtonian fluids has been successfully utilized to study viscosity changes on the nanoscale, many biomedically and technically relevant media exhibit non-Newtonian behavior. In particular, there are elastic components besides the viscous ones. As a consequence, the relationship between characteristic time constants, e.g. determinable by complex ac susceptibility (ACS), and material properties of the matrix becomes more complex. In this contribution we present different examples of nanorheological measurements utilizing ACS, magnetorelaxometry, and magneto-optical transmission. One example is the gelation process of aqueous gelatin solutions mixed with CoFe2O4 single-core MNP [1]. Gelatin solutions can be considered as a Voigt-Kelvin model system containing a viscous and an elastic term in parallel. The gelation process is monitored by ACS measurements at 23°C. An increase of viscosity manifests itself by a decrease of the peak frequency in the ACS imaginary part while an increase in shear modulus influences both the amplitude and the position of the maximum in the imaginary part. To analyze the measured ACS spectra, different models are applied and compared: the numerical model by Raikher et al. [2] and a phenomenological, modified Debye model. Whereas the dynamic viscosities obtained by fitting the models – extended by distributions of MNP diameters and viscosities – to the ACS spectra agree very well, the derived values for the shear modulus show the same temporal behavior during the gelation process but vary roughly by a factor of two. To verify the values for viscosity and shear modulus obtained from nanorheology, macrorheological measurements are in progress.

Financial support by the DFG via Priority Program 1681 (LU800/4-2, SCHM1747/10-2, TS62/4-2) is gratefully acknowledged.

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Magnetic Particle Nanorheology in Complex Fluids

M. Hermes (Universität zu Köln), E. Roeben (Universität zu Köln), L. Kibkalo (Universität zu Köln), A. Schmidt (Universität zu Köln) 17:50

Considering the rheology of materials, one can distinguish between the macroscopic examination of the (quasi-)continuous properties of bulk materials, and microscopic probing, where characteristics of the materials are related to the microstructure of the respective sample. Micro- or nanorheology is of particulate interest for the study of soft matter and biological systems, especially when spatial mechanical properties, interfaces or particle-matrix interactions are considered. In tis novel approach of magnetic particle rheology, small particles are used as probes, allowing the time-resolved analysis of the dynamic response of the magnetic nanoprobes to oscillating magnetic fields by means of dynamic susceptibility. For this purpose, we employ poly(ethylene oxide) (PEO) aqueous solutions as model systems with well-known characteristics in terms of molecular hydrodynamic radius, entanglement length, and mesh size. As magnetic probes, we employ well-defined, magnetically blocked CoFe2O4-nanoparticles, and their Brownian relaxation in the complex fluid is investigated by means of AC susceptometry between 1 Hz and 250 kHz. The use of different theoretical models gives access to the frequency-dependent complex viscosity and mechanical moduli from complex susceptibility data.[1] In addition to the PEO model systems, we investigate the dynamic behavior of reversible networks based on terpyridine-telechelic PEO star molecules and their metal cation complexes. In order to account for size effects, we systematically vary the hydrodynamic diameter of the probe particles by attachment of a silica shell with different thickness.

DFG-PP 4 : Field Controlled Particle Matrix Interactions: Synthesis Multiscale Modeling and Application of Magnetic Hybrid Materials

Wednesday 14:00 - 16:00 Coudraystr. 13B, 2nd floor, Room 210

A torsion pendulum experiment to study the rotational effect in ferrofluids with different concentrations of magnetic nanoparticles

A. Storozhenko (South West State University Kursk, Russia), R. Stannarius (Otto von Guericke University Magdeburg), K. May (Otto von Guericke University Magdeburg), T. Trittel (Otto-von-Guericke University Magdeburg) 14:00

The so-called rotational effect is a feature of nanostructured magnetic fluids which is manifested when an external rotating magnetic field is applied [1,2]. Our current contribution is devoted to the dependence of the rotational effect on the concentration of

magnetic nanoparticles in a ferrofluid as well as on the rheological properties of the carrier medium. The study has been conducted using an experimental setup presented previously [3]. In our torsion pendulum experiment, a ferrofluid sample is filled into a spherical glass container which is suspended on a thin glass fiber. The sample is placed in a rotating or oscillating magnetic field generated by two pairs of Helmholtz coils. We measure the torque density which is found from the accurate observation of the distortion of the glass fiber in dependence on the applied external magnetic field strength and frequency. For our experiments, we used commercial magnetic fluid APG 2135 from Ferrotec Corporation (Japan). The carrier liquid is synthetic hydrocarbon oil and the magnetic phase is magnetite. We diluted this magnetic fluid with durasyn to volume concentrations 50 %, 60 %, 70 %, 80%, 90 %, 100 %. These concentrations refer to the APG 2135 content. The results show a pronounced influence of the particle concentration as well as the rheological properties of the carrier medium on the rotational effect. We explain the results using a model that takes into account field-driven aggregation of the magnetic nanoparticles in stationary or slowly rotating fields. At sufficiently high rotation rates, the rotating magnetic field obviously destroys such aggregates, which results in a decreasing torque with increasing rotation frequency of the field. In addition to the aggregation phenomenon, the rotational effect is also influenced by the decreasing viscosity and changes of magnetic properties of the system as a consequence of the dilution with low-viscosity non-magnetic solvent.

Acknowledgements This study was funded by RFBR, Russia within research project No. 16-52-12035/16 and by DFG, Germany within Topical Program SPP 1681, Project STA 425/36.

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Field-induced plasticity of magneto-sensitive elastomers in context with soft robotic gripper applications

T. Kaufhold (Ilmenau University of Technology), J. Chavez-Vega (Ilmenau University of Technology), T. Becker (Ilmenau University of Technology), V. Böhm (Ilmenau University of Technology), K. Zimmermann (Ilmenau University of Technology), M. Martens (TU Braunschweig EMG), M. Schilling (TU Braunschweig EMG), T. Gundermann (Lehrstuhl für Magnetofluiddynamik, Mess- und Automatisierungstechnik, TU Dresden), S. Odenbach (Lehrstuhl für Magnetofluiddynamik, Mess- und Automatisierungstechnik, TU Dresden) 14:20

Magnetic hybrid composite materials have the peculiarity to change their mechanical properties when influenced by a magnetic field. This special characteristic can be used

to develop smart actuators, sensor systems and control mechanisms. In the paper the use of magneto-sensitive elastomers (MSE), composed of silicone rubber and silicone oil, with incorporated magnetic particles, in a form-fit gripper application is considered. The field-induced plasticity effect of MSE is used, to realise reversible recoverable shape adaptation of the gripper to the objects to be manipulated. The focus lies on the characterisation of the mechanical properties of the MSE for the specific application.

Interactions of Protein Coated Magnetic Nanoparticles with Biological Systems

A. Weidner, C. Gräfe (Universitätsklinikum Jena), M. von der Lühe, J. Clement, F. Schacher, S. Dutz (TU Ilmenau) 14:40

A protein corona is formed immediately on particles surface when magnetic nanoparticles (MNP) are exposed to the blood circulation. The aim of the here presented study was to analyze corona formation during in vitro serum incubation depending on the composition of the protein source and to investigate the interactions of these hybrid particles with living cells. We incubated cytotoxic polyethylenimine (PEI) coated MNP in defined mixtures of cell medium and fetal calf serum (FCS) for defined times and temperatures to obtain the protein coated MNP. Before and after the incubation the physical properties of the MNP were determined (zeta-potential, vibrating sample magnetometry, thermogravimetric analysis, transmission electron microscopy as well as sodium dodecyl sulfate polyacrylamide gel electrophoresis (SDS-PAGE)). Effects on cell viability were investigated for human brain microvascular endothelial cells (HBMEC) by the CellTiter Glo™ test and for long-term viability by real time cell analysis. The particle-cell interactions with HBMEC were studied by means of flow cytometry of fluorochrome-labelled particles. By means of investigation of zeta potential, SDS-PAGE, and thermogravimetry the influence of FCS concentration on the formation of the protein corona is clearly demonstrated. No cytotoxic effect of PEI-coated MNP was observed after protein corona formation. Similarly, long-term viability assays showed that the protein corona masks cytotoxic effects. Flow cytometry investigations indicated that FCS coating reduces the particle-cell interaction of cytotoxic PEI-coated MNP. Ongoing investigations focus on corona formation kinetics and in vitro and in vivo experiments on the biological fate of serum incubated MNP after cellular uptake.

This work is supported by Deutsche Forschungsgemeinschaft (DFG) in frame of priority programme 1681 (FKZ: CL202/3-2, DU 1293/4-2, SCHA1640/7-1).

In-vitro blood-brain barrier flow model to investigate the passage of magnetic nanoparticles

M. Liebl (Physikalisch-Technische Bundesanstalt (PTB)), C. Gräfe (Universitätsklinikum Jena), P. Radon (Physikalisch-Technische Bundesanstalt (PTB)), J. Clement (Universitätsklinikum Jena), F. Wiekhorst (Physikalisch-Technische Bundesanstalt (PTB)) 15:00

Magnetic nanoparticles (MNPs) open the way for novel cancer treatment approaches, in which they act as drug delivery agents in magnetic drug targeting or as heat generators

in magnetic hyperthermia. Currently, intense research is carried out on MNP mediated transport of therapeutics through the blood-brain barrier for treatment of brain disorders. Physical phantoms are often a mandatory prerequisite to simulate and investigate relevant parameters influencing the passage of MNPs through cell barriers, as e.g. the MNP concentration and coating, hydrodynamic and physical MNP properties, strength and application duration of the magnetic gradient field, physical flow properties and the interplay between cells and MNPs. Here, we present an approach of a phantom combining a closed-cycle flow system with online MNP quantification, defined magnetic gradient fields and a cell chamber mimicking a physiological blood brain barrier. A peristaltic pump drives the MNP suspension through a closed cycle silicon tube system connected to the cell chamber. A cube-shaped neodymium magnet (edge length of 9 mm) providing magnetic gradient fields up to 80 T/m for targeted MNP passage can be precisely positioning of the magnets mounting. For quantification this tube is directed through the pickup coil of our magnetic particle spectroscopy (MPS) device. MPS is based on the detection of the non-linear dynamic response of the MNPs' magnetization exposed to a harmonic excitation field of typical 25 mT amplitude and allows for sensitive quantification of MNP amounts with a detection limit of a few nanograms. Furthermore, MNP quantification within the MNP flow system is feasible even in opaque media like blood. Suitable tube materials were tested and chosen with regard to unwanted MNP binding and magnetic impurities. Promising MNP systems with different coatings as polyethylenimine (fluidMAG-PEI) or starch (fluidMAG-D, both chemicell GmbH Berlin), were preselected by in-vitro investigations of the binding behavior of MNP to human brain microvascular endothelial cells. Especially for the latter particle type, no cytotoxic or barrier-disrupting effects were detected during MNP incubation for up to 24h. However both cellular interaction and uptake of these starch-coated MNPs could be observed, thus allowing the transcellular particle passage across the biological barrier. Indeed, endpoint measurements performed with MPS already indicated a concentration- and time-dependent passage of fluidMAG-D through HBMEC layers under static conditions. However, flow conditions during cell cultivation can influence cellular physiology in different ways. With our approach a more physiologic barrier situation can be investigated with real time-resolution to provide a better insight into processes of the barrier-associated passage of MNPs.

This work was supported by the DFG priority program SPP1681 (CL202/3-2, WI4230/8-2)

DFG-PP 5: Calm, Smooth and Smart

Organizer: Peter Eberhard (University of Stuttgart)

DFG-PP 5 : Calm, Smooth and Smart

Wednesday 14:00 - 16:00 Coudraystr. 9A, Lecture hall 6

DFG Priority Programme SPP 1897: "Calm, Smoot and Smart – Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation" - an Overview

P. Eberhard (Uni Stuttgart - ITM), N. Walker (Uni Stuttgart - ITM) 14:00

Over the last few years, the concept of lightweight design has become more and more important in engineering. Herein, it is the aim to reduce the mass of any kind of technical structure to a minimum in order to save resources, costs and energy during both manufacturing and operation. Following the rules of this design principle often also means to make technical components and, thus, the overall system more sensitive to unwanted vibrations. These vibrations can cause severe environmental and health issues, and are, hence, to be minimized. Within the framework of the established priority programme entitled "Calm, Smooth and Smart – Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation" (SPP 1897), this yet inevitable dependence shall now be eliminated by developing novel approaches for influencing structural vibrations, leading to a "calm, smooth and smart" behaviour of technical units. To achieve this goals experts in the fields of mechanics, mathematics, control engineering, tribology, fluid mechanics and material science are working together.

Model Order Reduction for Parametric Nonlinear Mechanical Systems – State-of-the-Art and Future Research

C. Meyer (Chair of Applied Mechanics, Technical University of Munich), C. Lerch (Chair of Automatic Control, Technical University of Munich), B. Lohmann (Chair of Automatic Control, Technical University of Munich), D. Rixen (Chair of Applied Mechanics, Technical University of Munich) 14:20

Finite-element-analyses of advanced mechanical structures that undergo large deflections usually lead to high-dimensional systems of nonlinear equations. Their solution requires high computational effort which is crucial for design iterations, such as optimization or parameter studies. Nonlinear model order reduction methods are used to reduce these computational costs.

Similar to reduction methods for linear systems, the number of unknowns is reduced by projecting the displacements onto a subspace spanned by a reduction basis. In contrast to linear systems, nonlinear systems do not have eigenvectors which can be used as

reduction basis. For developing nonlinear reduction methods, it is a first challenge to determine a good reduction basis that is small but accurate.
A second challenge is to reduce computational costs for the evaluation of the nonlinear term. While in linear analyses the stiffness matrix can be simply reduced by matrix multiplications, in nonlinear analysis the nonlinear force vector has to be evaluated at every iteration step in the full element domain. In order to reduce these evaluation costs, hyperreduction methods are used.
This contribution gives an overview of state-of-the-art-methods for both basis-selection and hyperreduction.
Furthermore, we give an outlook on our future research within our project in the DFG Priority Program 1897 "Calm, Smooth and Smart Structures". It deals with the development of simulation-free hyperreduction techniques for parametric nonlinear mechanical systems.

Model reduction for finite element models of disk brakes

V. Mehrmann (TU Berlin), N. Gräbner (TU Berlin), S. Quraishi (TU Berlin), C. Schröder (TU Berlin), U. von Wagner (TU Berlin) 14:40

Numerical methods for model reduction in the numerical simulation of disk brake squeal are presented. Automotive disk brake squeal is a high frequency noise phenomenon based on self excited vibrations. Our new parameterized model reduction method is based on a variation of the proper orthogonal decomposition method and involves the solution of a large scale, parametric eigenvalue problem. Several important challenges arise, some of which can be traced back to the finite element modeling stage. Compared to the current industrial standard our new approach is more accurate in vibration prediction and achieves a better reduction in model size. This comes at the price of an increased computational cost for the off-line, but it still gives useful results when the classical modal reduction method fails to do so. We illustrate the results with several numerical experiments, some from real industrial models, some from simpler academic models.These results also indicate where improvements of the current black box industrial codes are advisable.

Nonlinear Multiple Body Models for Brake Squeal

S. Koch, N. Gräbner (TU Berlin), H. Gödecker, U. von Wagner (TU Berlin) 15:00

Brake squeal is a self-excited vibration with initially inclining amplitude reaching a limit cycle due to nonlinearities. For proper simulation of this behavior, it is necessary to know the origin and the influence of the brake system's nonlinearities. It is generally known, that nonlinearities are inherent to the joints [1,2], complex friction laws [3] and the friction material of the system [4]. In this work, the influence of friction material and shim nonlinearities on the existence of a limit cycle is investigated. Stiffness and damping characteristics are determined using the chair's owned DCTR test rig. It is shown, how nonlinear characteristics, which are necessary for simulation, are obtained from the performed measurements. They are incorporated in a multiple body model composed of

brake disk, pads, shims, carrier and caliper from which the nonlinear equations of motion are derived. For the investigation of the bifurcation behavior, the equations of motion are transformed into normal form [5]. It is then possible to describe the bifurcation behavior with respect to parameter influences. Ultimately, with this information it is possible to show the influence of the investigated nonlinearities on brake squeal. This work is funded by DFG, WA 1427/24-1 Literature [1] M. Tiedemann, S. Kruse and N. Hoffmann, „Dominant Damping Effects in Friction Brake Noise, Vibration and Harshness: the Relevance of Joints“, Proceedings of the Institution of Mechanical Engineers Part D: Journal of Automobile Engineering, 229. 6, pp. 728-734, 2014. [2] N. Gräbner, M. Tiedemann, U. von Wagner and N. Hoffmann, „Nonlinearities in Friction Brake NVH-Experimental and Numerical Studies“, SAE Technical Paper No. 2014-01-2511, 2014. [3] G.P. Ostermeyer, “On the dynamics of the friction coefficient”, Wear, 254.9, pp 852-858, 2003. [4] S. Hornig and U. von Wagner, „Experimental Identification of Brake Lining Material Properties Subjected to Combined Static and High Frequency Loading-A Step Towards a Better Prediction of Disc Brake Squeal“, SAE Technical Paper No. 2011-01-2353, 2011. [5] D. Hochlenert. ”Nonlinear stability analysis of a disk brake model.” Nonlinear Dynamics 58.1-2, pp 63-73, 2009.

Experimental investigations of brake pad shim properties

D. Schmid (TU Berlin), N. Gräbner (TU Berlin), U. von Wagner (TU Berlin) 15:20

Brake squeal on automotive disk brakes represents a high frequency noise phenomenon resulting in potential customer complaints. The avoidance of squeal causes high costs in the automotive industry worldwide. One countermeasure against this disruptive noise issue is the application of damping shims bonded to backplates of brake pads. Shims are thin composite structures consisting of viscoelastic rubber layers and metal plates with high stiffness. The selection of appropriate shims is according to the state of the art mainly based on trial and error. Current approaches seem to map the effects of shims on brake squeal insufficiently. To describe the shim behavior in an improved manner, prior experimental investigations have to be carried out, focusing on the identification of modal damping and stiffness values. Corresponding results are presented here.

The contribution shows experimental results of shims firmly bonded to brake pads and rectangular steel plates. One emphasis is to enhance the determination and evaluation method of damping factors. Temperature variations and the analysis of nonlinearities like various exciting forces are examined in detail. As a result, the general influence of shims is presented and compared to measurements without damping materials.

This work is funded by DFG, WA 1427/27-1, within the SPP 1897 “Calm Smooth and Smart - Novel Approaches for Influencing Vibrations by Means of Deliberately Introduced Dissipation“.

DFG-PP 5 : Calm, Smooth and Smart

Wednesday 16:30 - 18:30 Coudraystr. 9A, Lecture hall 6

Predicting the Influence of an Added Liquid in a Particle Damper using Coupled SPH and Discrete Element Method

C. Gnanasambandham (University of Stuttgart), P. Eberhard (University of Stuttgart) 16:30

Particle dampers are a promising alternative compared to conventional dampers due to their very flexible ability to dissipate energy in a wide frequency range also in rough environments. Simultaneously they cover additional functions like load bearing and noise reduction. For the understanding of particle dampers it is important to take into account the relevant physical phenomena which are interacting. The particles are modeled using the Discrete Element Method (DEM). Mesh-free methods such as DEM pose to be appropriate in modeling large displacements of particle fillings in the damper and the dynamic contacts between adjacent particles resulting from high dynamics. In this work, a numerical experiment, where a particle damper is attached to a vertical leaf-spring, is set up to investigate the influence of typical parameters such as particle fill-ratios, particle size, material properties, and enclosure shapes on the damping performance of the particle damper. Moreover, the effect of an added liquid is also investigated. The Smoothed Particle Hydrodynamics (SPH) method is used in order to model the motion of the fluid. By using a coupled SPH-DEM approach, it is shown that complex interactions between particle-fillings, liquid, and enclosure geometry can be sufficiently modeled. Thereby, it is possible to predict the influence of an added liquid on the vibration at tenuation properties of the particle damper.

NUMERICAL STUDY ON SHAPE FUNCTIONS FOR OPTIMAL EXPLOITATION OF THE ACOUSTIC BLACK HOLE EFFECT

S. Rothe (TU Braunschweig, Institut für Konstruktionstechnik), M. Dorn (TU Braunschweig, Institut für Konstruktionstechnik), S. Langer (TU Braunschweig, Institut für Konstruktionstechnik) 16:50

The acoustic black hole effect offers a great possibility to damp a whole construction in a very efficient way. The main idea of this approach is to weaken thin structures locally to concentrate the structure-borne sound in this area. Therefore material is removed in a certain region, which is referred to as an acoustic black hole. This measure leads to a focusing of acoustically critical bending waves. By applying a damping measure, e.g. constraint layer damping, within the acoustic black hole, the structure is globally damped by a local measure.

The shape function of an acoustic black hole is a major issue for optimizing the efficiency of damping. The material diminution, equivalent to the reduction of the mechanical impedance, has to be smooth in order to avoid reflection of bending waves. In literature

a power function with a higher order than two is recommended. Focusing the structure-borne sound works better by increasing the order. In consideration of the limit case – infinite order, equivalent to an impedance step – there must be an optimum between these to borders in acoustical sense.

In this paper numerical studies are carried out to delimit the optimal order for a power function approach as shape function of an acoustic black hole. For this purpose a beam as a generic structure is used. In addition, alternative function approaches are investigated and compared.

Characterization of complex states for friction-excited systems

M. Stender (Hamburg University of Technology), M. Tiedemann (AUDI AG Ingolstadt), N. Hoffmann (Imperial College London) 17:10

For many engineering structures the dynamical response during operation is rarely stationary or regular. In fact, many studies on measured data reveal the irregular nature of dynamical system responses, for example in the field of research on brake squeal. Therefore, linear measures, such as amplitude and frequency spectra, cannot characterize the core dynamics contained in an irregular time series. Additionally, linear methods for damping extraction from measured signals tend to lose significance when it comes to irregular responses of self-excited systems. This work aims at highlighting the need for quantifiers from nonlinear time series analysis to adequately characterize real-world vibration data. In a first step a minimal model is studied to relate nonlinear time series quantifiers to internal system states and dissipation considerations. The goal of this research is to develop an understanding for the information contained in measured time series data concerning dissipation mechanisms of complex friction-excited systems.

On the Dynamics of a Lock-up Mass Damper

A. Fidlin (Karlsruhe Institute of Technology (KIT)) 17:30

Dynamics of a classical mass damper locked-up by a dry friction element is investigated both using asymptotic methods and numerical simulations. It is assumed that the mass of the mass damper is much smaller than the mass of the main system. Consequently the non-dimensional sliding friction force is small in the equations for the main system, but not small in the equation for the mass damper. In order to obtain the approximate analytic solution for this equation, a special procedure has been developed, based on the averaging for strongly damped systems [1]. It can be shown that the obtained solution for the mass damper itself is valid in the vicinity of the main resonance without any assumptions on the magnitude order of friction and excitation forces. Subsequently the approximate solution can be obtained for the amplitude of the main mass. It can be shown that the considered mass damper can limit the amplitude of the main mass in a wide range of parameters without any viscous damping. In this sense its effect is very similar to that of the sequential friction-spring damper [2]. It doesn't dissipate any energy is the vibrations amplitude is sufficiently small (due to sticking in the lock-up

friction) and starts to slide and to dissipate energy if necessary. However the advantage of the current solution is that it can be used as an add-on element which is not necessarily integrated in the main structure. It can be attached to the structure as an additional component if necessary. All the effects can be confirmed by the numerical simulations of the system. [1] A. Fidlin and O. Drozdetskaya: On the averaging in strongly damped systems: the general approach and its application to asymptotic analysis of the Sommerfeld effect, Procedia IUTAM 18 (2016), pp. 43 – 52. [2] A. Fidlin, M. Lobos: On the limiting of vibrations amplitudes by a sequential friction-spring element. Journal of Sound and Vibration 333 (2014), pp. 5970 – 5979.

DFG-PP 6: Non-smooth and Complementary-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

Organizer: Michael Hintermüller

DFG-PP 6 : Non-smooth and Complementary-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

Thursday 14:00 - 16:00 Coudraystr. 11C, Room 101

SPP 1962: Non-smooth and Complementarity-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

M. Hintermüller 14:00

Non-differentiable structures and partial differential operators arise naturally in numerous problems in the applied sciences, leading to non-smooth distributed parameter systems. This non-smoothness may materialize in the formulation of the problem itself, in inequality constraints or complementarity systems, or as a result of competition and hierarchy. Some applications where such non-smoothness arises are quasivariational inequalities, generalized Nash equilibrium problems and mathematical programs with equilibrium constraints. This talk will describe the main goals of the program, present some of the model problems where non-smoothness is inherent, and outline its consequences on the resulting mathematical and numerical analysis. The talk will also touch on the crucial idea of transitioning from smoothing or simulation-based approaches to genuinely non-smooth and modern techniques to deal with the problems. Some recent advances in the field will also be presented.

Strong stationarity conditions for the optimal control of a Cahn-Hilliard-Navier-Stokes system

T. Keil, M. Hintermüller 14:20

This talk is concerned with the optimal control of two immiscible fluids with non-matched densities. For the mathematical formulation of the fluid phases, we use a coupled Cahn-Hilliard/Navier-Stokes system which has recently been introduced by Abels, Garcke and Grün in [1]:

$$\partial_t \varphi + v\nabla\varphi - \mathrm{div}(m(\varphi)\nabla\mu) = 0, \tag{4.1}$$

$$-\Delta\varphi + \partial\Psi_0(\varphi) - \mu - \kappa\varphi = 0, \tag{4.2}$$

$$\partial_t(\rho(\varphi)v) + \mathrm{div}(v \otimes \rho(\varphi)v) - \mathrm{div}(2\eta(\varphi)\epsilon(v)) + \nabla p + \mathrm{div}(v \otimes J) - \mu\nabla\varphi = 0, \tag{4.3}$$

$$v_{|\partial\Omega} = \partial_n\varphi_{|\partial\Omega} = \partial_n\mu_{|\partial\Omega} = 0, \tag{4.4}$$

$$\mathrm{div}v = 0, (v,\varphi)_{|t=0} = (v_a, \varphi_a). \tag{4.5}$$

The free energy density Ψ_0 associated with the underlying Ginzburg-Landau energy in the Cahn-Hilliard system is given by the double-obstacle potential. As a consequence, the system (4.1)-(4.2) becomes a variational inequality of fourth order.
We propose a suitable time discretization for the above system and verify the existence of solutions to the semi-discrete Cahn-Hilliard/Navier-Stokes system.
The optimal control problem is formulated by introducing an appropriate objective functional and a distributed control u which enters the Navier-Stokes equation (4.3) on the right-hand side.
We establish the existence of optimal controls and further investigate the sensitivity of the associated control-to-state operator verifying a Lipschitz estimate. A characterization of the directional derivative of the constraint mapping is provided involving a system of variational inequalities and equations.
Finally, we present strong stationarity conditions for the optimal control problem which are derived via an variational approach pioneered by Mignot and Puel, cf. [2].

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Efficient Methods for Optimization in Shape Spaces

K. Welker (Trier University), V. Schulz, M. Siebenborn (Trier University) 14:40

Shape optimization problems arise frequently in technological processes which are modelled in the form of partial differential equations (PDEs). In many practical circumstances, the shape under investigation is parametrized by finitely many parameters, which on the one hand allows the application of standard optimization approaches, but on the other hand limits the space of reachable shapes unnecessarily. Shape calculus

presents a way out of this dilemma. Major effort in shape calculus has been devoted towards expressions in so-called Hadamard-forms, i.e., in forms of integrals over the surface of the shape under investigation. It is often a very tedious process to derive such surface expressions. Along the way, there appear volume formulations in the form of integrals over the entire domain as an intermediate step. In this talk, domain integral formulations of shape derivatives are coupled with optimization strategies on shape spaces. Efficient shape algorithms reducing analytical effort and programming work are presented. In this context, a novel shape space is proposed.

The limiting normal cone in Lebesgue and Sobolev spaces

F. Harder (TU Chemnitz), P. Mehlitz (TU Bergakademie Freiberg), 15:00
G. Wachsmuth (TU Chemnitz)

The limiting normal cone, which is also denoted as Mordukhovich normal cone, is a central concept in modern variational analysis. It allows to derive optimality conditions for finite-dimensional nonsmooth optimization problems under very low regularity requirements. In particular, it is applicable to mathematical programs with complementarity constraints (MPCCs), and one obtains optimality conditions of M-stationary type.
However, there literature concerning the limiting normal cone in infinite-dimensional spaces is scarce. In this talk, we are going to characterize the limiting normal cone in two important infinite-dimensional applications. First, we consider so-called decomposable sets (i.e., sets with pointwise constraints) in Lebesgue spaces and we are able to give a precise characterization of their normal limiting cone. Second, we study the complementarity set in Sobolev spaces.
The analysis in both situations is delicate and this is mainly induced by the fact that the limiting normal cone is, in general, not closed.

DFG-PP 6 : Non-smooth and Complementary-based Distributed Parameter Systems: Simulation and Hierarchical Optimization

Thursday 16:30 - 18:30 Coudraystr. 11C, Room 101

POD-based Set Oriented Multiobjective Optimal Control

D. Beermann (University of Konstanz), S. Peitz (Paderborn University), 16:30
S. Volkwein (University of Konstanz), M. Dellnitz (Paderborn University)

In a wide range of applications one is interested in optimally controlling a dynamical system with respect to concurrent, potentially competing goals. This gives rise to a multiobjective optimal control problem (MOCP):

$$\min_{y\in Y, u\in U} J(y,u) = \min_{y\in Y, u\in U} \begin{pmatrix} J_1(y,u) \\ \vdots \\ J_k(y,u) \end{pmatrix} \quad \text{s. t.} \quad \dot{y} = F(y,u),$$

where u is the control and y is the system state for which the dynamical behavior is described by F.
In the presence of multiple objectives, the set of optimal compromises, the so-called *Pareto set*, has to be approximated – in contrast to classical optimization problems, where one single optimal solution is computed. There exist various approaches to address MOCPs such as scalarization techniques, evolutionary algorithms or set oriented approaches. All of these have in common that a large number of function evaluations is typically required. Thus, the direct computation of the Pareto set can quickly become numerically infeasible. This is especially the situation when the dynamical system at hand is costly to solve, as is the case for problems described by (nonlinear) partial differential equations (PDEs).
Standard optimization methods for PDEs often make use of a discretization by finite elements or finite volumes which results in a high-dimensional system of ordinary differential equations. In a multi query context such as optimization or parameter identification, this approach often exceeds the limits of today's computing power and hence, a significant reduction of the computational cost is required. This can be achieved by approximating the PDE by a reduced order model (ROM) of low dimension, where models obtained by Proper Orthogonal Decomposition and Galerkin projection [1] have proven to be well-suited for nonlinear problems.
In this presentation we extend previous results on PDE-constrained multiobjective optimization using reduced order models. In [2], set oriented approaches were utilized to solve multiobjective optimal control problems governed by the Navier-Stokes equations using a pre-computed ROM. In [3] and [4], scalarization techniques were applied to semilinear PDE-constrained problems and error bounds were derived. In order to so solve problems with a larger number of objectives and to address non-smooth problems in the future, we combine these results and extend a set oriented algorithm with uncertainties [5] to PDE-constrained problems using POD-based ROMs with error estimates for the cost function and the gradients.

[1] P. Holmes, J. L. Lumley, G. Berkooz. *Turbulence, coherent structures, dynamical systems and symmetry.* Cambridge university press, 1998.

[2] S. Peitz, S. Ober-Blöbaum, M. Dellnitz. *Multiobjective Optimal Control Methods for Fluid Flow Using Reduced Order Modeling.* arXiv:1510.05819, 2015.

[3] L. Iapichino, S. Ulbrich, S. Volkwein. *Multiobjective PDE-Constrained Optimization Using the Reduced-Basis Method.* `http://kops.uni-konstanz.de/handle/123456789/25019`, 2013.

[4] S. Banholzer, D. Beermann, S. Volkwein. *POD-Based Bicriterial Optimal Control by the Reference Point Method.* 2nd IFAC Workshop on Control of Systems Governed by Partial Differential Equations, pp. 210–215, 2016.

[5] S. Peitz, M. Dellnitz. *Gradient-Based Multiobjective Optimization with Uncertainties.* arXiv:1612.03815, 2016.

Towards MOR for multiphase flows with variable densities governed by diffuse interface models with nonsmooth energies

M. Hinze (Universität Hamburg), C. Gräßle (Universität Hamburg) 16:50

We develop, implement and analyse reduced order models for multiphase flows with variable densities governed by the Cahn Hilliard/Navier-Stokes system with a nonsmooth free energy. Special emphasis is taken on the treatment of adaptively obtained spatial snapshots, and on the resolution of the nonlinearity introduced through the nonsmooth free energy.
This is joint work with Carmen Gräßle, Fachbereich Mathematik, Universität Hamburg

Optimal Control for Fracture Propagation Modeled by a Phase-Field Approach

I. Neitzel (Rheinische Friedrich-Wilhelms-Universität Bonn), T. Wick (École Polytechnique), W. Wollner (TU Darmstadt) 17:10

We are concerned with an optimal control problem governed by a fracture model using a phase-field technique. To avoid the non-differentiability due to the irreversibility constraint, the fracture model is relaxed using a penalization approach. Due to the removal of L^∞ bounds on the phase-field, well posedness of the penalized fracture model needs to be analyzed. Existence of a solution to the penalized fracture model is shown and utilized to establish existence of at least one solution for the regularized optimal control problem.

DFG-PP 7: Polymorphic Uncertainty Modeling for the Numerical Design of Structures

Organizer: Michael Kaliske (TU Dresden)

DFG-PP 7 : Polymorphic Uncertainty Modeling for the Numerical Design of Structures

Thursday 14:00 - 16:00 Coudraystr. 9A, Lecture hall 6

Polymorphic Uncertainty Modeling for the Numerical Design of Structures (SPP 1886)

M. Kaliske (TU Dresden) 14:00

Advanced engineering solutions are characterized by inherent robustness and flexibility as essential features for a faultless life of structures and systems under uncertain and changing conditions. An implementation of these features in a structure or system requires a comprehensive consideration of uncertainty in the model parameters and loads

as well as other types of intrinsic and epistemic uncertainties.
Numerical design of structures/systems should be robust with respect to uncertainties inherently present in resistance of materials, boundary conditions e.g. environmental and man imposed loads, physical and numerical models. This requires in turn the availability of a reliable numerical analysis, assessment and prediction of the lifecycle of a structure/system taking explicitly into account the effect of the unavoidable uncertainties.
Challenges in this context involve, for example, limited information, human factors, subjectivity and experience, linguistic assessments, imprecise measurements, dubious information, unclear physics etc. Due to the polymorphic nature and characteristic of the available information both probabilistic and set-theoretical approaches are relevant for solutions.

Comparison of nested collocation and projection algorithms for mixed aleatory and epistemic uncertaintites using a probability-box approach

A. Fau (Leibniz Universität Hannover), M. Dannert (Leibniz Universität Hannover), M. Broggi (Leibniz Universität Hannover), U. Nackenhorst (Leibniz Universität Hannover), M. Beer (Leibniz Universität Hannover) 14:20

Most numerical models for engineering applications include some uncertainties caused for example, by load, geometry or material properties. Two types of uncertainties may be distinguished, aleatory uncertainties due to random phenomena and epistemic uncertainties due to a lack of knowledge or data [1]. Input variables have generally both, aleatory and epistemic uncertainties. To model such mixed uncertain variables, probability bounds analysis has shown to be useful. The probability of an event is here not described by a unique function [2] but within an upper and a lower bound, which form a so-called probability-box (p-box) distribution function. One key issue in the applications is numerical effort [3]. Therefore, collocation and projection methods are proposed to improve numerical efficiency.
In this work, a stochastic finite element analysis for an elasto-plastic problem involving uncertain constitutive parameters is implemented. The underlying random field is modelled by a p-box. A nested collocation scheme, where samples are chosen within a certain lattice construction [4], and a projection method [5] are examined in a comparative study. The algorithms are tested with one- and two-dimensional example and verified by Monte Carlo simulation. A critical review of the two methods for mixed uncertainties description will be proposed in this contribution.

[1] A. Der Kiureghian and O. Ditlevsen. “Aleatory or epistemic? Does it matter?” Structural Safety, 31(2), pp. 105-112, 2009.
[2] S. Ferson and J. Hajagos.“Arithmetic with uncertain numbers: rigorous and (often) best possible answers”, Reliability Engineering and System Safety, 85(1-3), pp. 135-152, 2004.
[3] H. Zhang et al. *Structural reliability analysis on the basis of small samples: An*

interval quasi-Monte Carlo method, Mechanical Systems and Signal Processing, 37(1-2), pp. 137-151, 2013.
[4] D. Xiu and J. S. Hesthaven. *High-Order Collocation Methods for Differential Equations with Random Inputs.* SIAM J. Sci. Comput., 27(3), pp. 1118-1139, 2005.
[5] O.P. Le Maître and O.M. Knio. *Spectral Methods for Uncertainty Quantification*, Chap. *Non-intrusive Methods.* Springer, 2010.

On uncertainty in friction measurements

G. Ostermeyer (Technische Universität Braunschweig), M. Mueller (Technische Universität Braunschweig), T. Srisupattarawanit, A. Völpel 14:40

In the fields of mechanical engineering, friction is ubiquitous. It is a fundamental cause of energy loss and wear. Another concern is the occurrence of comfort-relevant friction induced vibrations. Prominent examples of this are NVH phenomena such as brake squeal, which is being investigated at great expense by the German automotive industry and academia, to determine its causes and potential influencing factors.
For this purpose, numerous specialized measurements are performed, and models of varying complexity are used. All of these measurements and models have the common trait that the coefficient of friction, defined as the ratio of the tangential force and normal force, has a decisive influence on the systems' stability.
To parameterize the friction coefficient in macroscopic models, measurements must be performed. In this case, often an average over time and over various loading procedures is used. As the measurements reveal, the coefficient of friction is in reality not constant, but is subject to a high degree of dynamics on various time scales, caused by complex processes in the boundary layer. A treatment of the coefficient of friction as a steady-state parameter, or even as a constant, is thus a major reduction.
The large variability of the coefficient of friction causes a corresponding variance in the stability limits of the models considered. This phenomenon is observed in the real world, where squealing seems to have a non-deterministic behavior. This suggests uncertainties in the modeling of the friction coefficient. Due to the various types of uncertainty (variability, incompleteness and inaccuracy), the entire problem is a matter of polymorphic uncertainty.
This paper focuses on the modeling of the friction coefficient, taking into account the various causes of uncertainty. Selections of raw data obtained at the authors institute throughout many years of research on friction phenomena in brake systems will be evaluated and classified with respect to its uncertainty properties.

Polymorphic Uncertainty Modeling of Heterogeneous Thermo - Hydro - Mechanical Coupled Systems under Vague Assumptions on Parameter Correlations

T. Lahmer (Bauhaus-Universität Weimar), C. Könke (Bauhaus-Universitaet Weimar), L. Nguyen-Tuan (Bauhaus-Universität Weimar), A. Schmidt 15:00

New hybrid materials and constructions with heterogeneous material properties gain in-

creasing importance due to the development of new light-weight building concepts. Furthermore, many natural and technical materials applied show a heterogeneous material distribution in the existing engineering constructions. Examples are typical geoscience materials or aggregate-matrix materials w.r.t their meso- and microscopic treatment in a multi-scale approach. The modeling of the material behavior during forecast simulations can either be done by the estimation of upper and lower bounds or by the application of multi-dimensional random fields. In multi-field situations, e.g. coupled thermal-hydro-mechanical systems like dams, dikes or subsoil deposits, there are a series of sensitive material properties which can be modeled via random fields. Often, these fields exhibit a certain correlation, e.g. in regions of deteriorated material the hydraulic permeability might be increased while the mechanical stiffness and strength is reduced. The question arising is, if this has also effects on other material properties and how the interdependency can be taken effectively into consideration in this case. In the given research, a methodology is derived which allows, based on a polymorphic uncertainty model, the generation of random fields for multi-physic applications, where however, the degree of interdependence of the different fields and their model parameters is not fully known. Therefore, the talk comprises first steps in the the development, analysis and application of a polymorphic uncertainty model, which captures the random variability of the material properties with vague information concerning their correlations and correlation lengths. First simulations for simplified THM models will be presented. The talk will also give some conclusions about the assessed structural reliability while using the newly proposed method.

On Using Fuzzy Arithmetic in Optimization Problems with Uncertain Constraints

M. Mäck (University of Stuttgart), M. Hanss (University of Stuttgart) 15:20

In engineering problems it is often required to not only find an optimal solution, but also to ensure that the solution is robust with respect to potential uncertainties. Existing algorithms for optimization deliver accurate solutions for a multitude of problems and a broad field of applications. A proper functioning of these algorithms, however, requires the provision of exactly known parameters, and thus, the availability of a detailed knowledge of the considered system as well as its potential restrictions and constraints. In reality, however, the model parameters might be uncertain and the constraints might be vaguely defined or even unknown, making the determination of an optimal and preferably robust solution very challenging. This deficiency of knowledge about the system is often referred to as uncertainty of epistemic type and it cannot be handled satisfactorily by methods of traditional probability theory, as used for uncertainty of aleatoric type. In contrast, possibilistic approaches, such as fuzzy arithmetic, prove well suited to represent uncertainty caused by incomplete information or deficient knowledge and to quantitatively analyze systems with epistemic uncertainties.
In this contribution, a general approach is presented where fuzzy arithmetic is used to tackle optimization problems with uncertain constraints. Based on the fuzzy arithmetical formulation, a special robustness criterion can be defined which allows for the determina-

tion of an optimal solution in due consideration of uncertain, fuzzy-valued constraints. Additionally, uncertain model parameters can be considered, leading to fuzzy-valued parameters also in the objective function, and thus, extending the methodology to a generalized approach to optimization under miscellaneous uncertain conditions. The potentials and drawbacks of the approach are discussed and illustrated on the basis of a meaningful example.

Solution Space approach to address polymorphic uncertainties in early phase structural design

F. Duddeck (Technische Universität München) 15:40

The main uncertainties encountered in early phase structural design are epistemic, i.e. they relate to lack of knowledge w.r.t. design decisions made later in the development process. Assessments of structural concepts are required based a partial knowledge of structural layouts of the relevant components. The solution space approach enables now a decoupled development of components assuring the overall fulfillment of design criteria. This is achieved by (i) establishing a simplified model for complete structural performances, (ii) evaluations using this simplified model to derive requirements for components, and (iii) optimizing these component requirements for maximal flexibility. This flexibility offers a lack-of-knowledge approach for epistemic uncertainties where single components can be developed allowing modifications of components later in the development process without endangering the overall concept behavior. The optimization w.r.t. flexibility is then followed by structural optimizations (e.g. size, shape and topology) where further uncertainties (aleatoric) can be considered. A polymorphic uncertainty approach can be realized combining different robustness methods for epistemic and aleatoric uncertainties. The approach was originally introduced and further developed for crashworthiness and then extended to driving dynamics. New developments, mainly for crashworthiness, will be presented in this paper addressing approaches for reduction of complexity related to multi-load case optimization, optimized communality of several vehicles and computational efficiency. The approach is based on Solution Spaces using decoupled corridors (upper and lower limit) for force-displacement curves for each component. Structural shape and topology optimization is then used in an exemplary manner to illustrate the method with particular focus on load case, material, and geometry uncertainties. An outlook will be given concerning generalization of the approach to other disciplines.

DFG-PP 7 : Polymorphic Uncertainty Modeling for the Numerical Design of Structures

Thursday 16:30 - 18:30 Coudraystr. 9A, Lecture hall 6

Polymorphic uncertainty quantification for stability analysis of fluid saturated soil and earth structures

C. Henning, T. Ricken (TU Dortmund University) 16:30

Nowadays, numerical simulations enable the description of mechanical problems in many application fields, e.g. in soil or solid mechanics. During the process of physical and computational modeling, a lot of theoretical model approaches and geometrical approximations are sources of errors. These can be distinguished into aleatoric (e.g. model parameters) and epistemic (e. g. numerical approximation) uncertainties. In order to get access to a risk assessment, these uncertainties and errors must be captured and quantified. For this aim a new priority program SPP 1886 has been installed by the DFG which focuses on the so called polymorphic uncertainty quantification. In this subproject, which is part of the SPP 1886 (sp12), the focus is driven on quantification and assessment of polymorphic uncertainties in computational simulations of earth structures, especially for fluid-saturated soils. To describe the strongly coupled solid-fluid response behavior, the theory of porous media (TPM) will be used and prepared within the framework of the finite element method (FEM) for the numerical solution of initial and boundary value problems [1, 2]. To capture the impacts of different uncertainties on computational results, two promising approaches of analytical and stochastic sensitivity analysis will enhance the deterministic structural analysis [3, 4, 5]. A simple consolidation problem already provided a high sensitivity in the computational results towards variation of material parameters and initial values. The variational and probabilistic sensitivity analyses enable to quantify these sensitivities. The variational sensitivities are used as a tool for optimization procedures and capture the impact of different parameters as continuous functions. An advantage is the accurate approximation of the solution space and the efficient computation time, a disadvantage lies in the analytical derivation and algorithmic implementation. In the probabilistic sensitivity analysis from the field of statistics, the expense only increases proportionally to the problems dimension. Instead of a constant value, the model parameters are defined as probability distribution, which provides random values. Thus, a set of solution data is built up by several cycles of the simulation. Different approaches of the Bayes statistics will enable to receive accurate information with just a few simulations. The overall objective is the development of more efficient methods and tools for the sizing of earth structures in the long-run.

[1] R. De Boer: *Theory of Porous Media*, Springer, New York, 2008.

[2] W. Ehlers and J. Bluhm: *Foundations of multiphasic and porous materials*, Porous

Media: Theory, Experiments and Numerical Applications, pages 3-86., Springer-Verlag, 2002.

[3] F.-J. Barthold: *Theorie und Numerik zur Berechnung und Optimierung von Strukturen aus isotropen, hyperelastischen Materialien* Technische Universität Braunschweig, Forschungs- und Seminararbeit aus dem Bereich Mechanik der Universität Hannover, Bericht-Nr. F 93/2, 1993.

[4] J. Stieghan: *Variationelle Sensitivitätsanalyse in der Theorie poröser Medien* Technische Universität Carolo-Wilhelmina zu Braunschweig, 2008.

[5] J. E. Oakley and A. O'Hagan: *Probabilistic sensitivity analysis of complex models: a Bayesian approach*, J. R. Statist. Soc. B, 66(3):751-769, 2004.

Multivariate stochastic finite element method with correlated material parameters

E. Penner (Paderborn University), I. Caylak (Paderborn University), R. Mahnken (Paderborn University) 16:50

It is well known that material properties are uncertain due to the manufacturing process or the heterogeneity. In addition, there are measurement errors and incomplete information on material properties, geometry and boundary conditions. These uncertainties also lead to uncertainty in the mechanical response. Therefore continuum modeling, where input parameters of the stochastic model are uncertain, should be designed by a stochastic partial differential equation (SPDE) instead of a deterministic PDE. A possible numerical method for solving the SPDEs is the stochastic finite element method (SFEM), where the Monte Carlo (MC) method or polynomial chaos expansion (PCE) as presented in [1] for small deformation problems, are commonly used.
The key idea of our contribution is to consider the uncertainty in material parameters by modeling them as multivariate stochastic variables. Furthermore, a statistical analysis of the random material parameters including their correlations is performed. Usually, the material parameters are considered as stochastically independent. However, in our work we consider the dependency including the correlation obtained from experimental data. The multivariate stochastic variables, in our case the material parameters, are formulated in the multivariate PCE. In order to determine the corresponding PC coefficients for correlated stochastic material parameters, we use the Cholesky decomposition.
In a numerical example we consider the static problem for uniaxial tension of a rectangular plate. This problem is investigated under a plane stress state in order to represent exactly the experimental setup conditions. Based on experimental data, statistics are generated for material parameters. Then, PC coefficients are calculated and a multivariate stochastic finite element analysis is performed. Finally, the probability density functions of the system response of simulation and experiment are compared with each other.

[1] R. G. Ghanem and P. D. Spanos, *Stochastic Finite Elements: A Spectral Approach,* Springer-Verlag, New York, 1991.

A possibilistic evaluation using Fuzzy finite element method based on sparse experimental data

A. Dridger (Paderborn University), I. Caylak (Paderborn University), R. Mahnken (Paderborn University) 17:10

In many engineering applications the uncertainty quantification has become important in order to obtain authentic results using, e.g. the stochastic finite element method (SFEM). Generally, the corresponding partial differential equations (PDEs) are subjected with different kinds of uncertainties, e.g. in material parameters, in boundary conditions or in the geometry. The uncertainties may arise from linguistic, imprecise, incomplete or statistical properties and are categorized into aleatoric and epistemic types. The aleatoric uncertainties may be described by stochastic methods characterized by randomness, whereas epistemic uncertainties may be described by the fuzzy approach using fuzzy sets and/or membership functions [1], respectively.
In this work we investigate the combination of aleatoric and epistemic uncertainties called "imprecise probabilities" [2], for linear elastic continua. For this reason, a membership function is characterized as a "possibility distribution" which encode a family of probability distributions. The associated probability density functions are transformed into possibility distributions using the probability-possibility transformation [3]. The main objective is the numerical computation of the solution considering the interaction of corresponding fuzzy parameters. Possibilistic evaluation of the fuzzy finite element method (FFEM) is presented. The α-level discretization technique [1] is applied in order to reduce the fuzzy arithmetic based FEM to an interval arithmetic based FEM. In this context, our method is applied in a numerical example for a plate with a ring hole.

[1] B. Moeller and M. Beer, *Fuzzy Randomness - Uncertainty in Civil Engineering and Computational Mechanics,* Springer, 2004.

[2] D. Dubois and H. Prade, *Possibility Theory and Its Applications: Where Do We Stand?* Springer, pp. 31-60, 2015.

[3] M. Hamed and M. Serrurier, *Representing uncertainty by possibility distributions encoding confidence bands, tolerance and prediction intervals,* Springer, pp. 233-246, 2012.

5 Poster Session

Tuesday and Wednesday — Weimar hall, Foyer
11:00 - 11:30
Organizers: Dominik Kern (TU Chemnitz)
Melanie Todt (TU Wien, Institute of Lightweight Design and Structural Biomechanics)

Variational Integrators for Standard and Non-standard Heat Transfer

D. Kern (TU Chemnitz), J. Blomberg Ghini (Conseil Européen pour la Recherche Nucléaire (CERN))

Variational Integrators, sometimes referred to as symplectic integrators, were originally developed for conservative mechanical systems. Their advantages motivated further extensions, i.a. for simulations of thermomechanical systems.
The standard heat transfer by Fourier's law is not conservative. Therefore it needs to be included by D'Alembert terms. This kind of heat transfer leads to the classical, parabolic heat equation.
Whereas non-standard heat transfer of Green & Naghdi type II fits well into the variational framework, as it directly enters the variational formulation via the free energy. The resulting partial differential equation is hyperbolic.
In this contribution we focus on the nonstationary thermal problem and derive a variational integrator that covers both, Fourier's law as well as Green & Naghdi type II. A one-dimensional continuum, a bar, serves as model problem for both kinds of heat transfer.

High performance optimization algorithms for interface identification problems

M. Siebenborn (Trier University)

This poster presents optimization approaches for large scale interface identification problems prepared for supercomputers. In many applications, which are modeled by partial differential equations, there is a small number of spatially distributed materials or parameters separated by interfaces. Often these interfaces form complex contours forcing high resolutions in the discretization schemes. The challenge is thus to combine HPC techniques with shape optimization in order to come up with scalable algorithms even for very large problems. This can be achieved by a combination of multigrid strategies and quasi Newton methods. It is also shown how different shape metrics affect the quality of finite element meshes and which are the most suitable ones.

Shell-based ply-level models of layered composites

M. Todt (TU Wien, Institute of Lightweight Design and Structural Biomechanics), M. Schwab (TU Wien, Institute of Lightweight Design and Structural Biomechanics), F. Rammerstorfer (TU Wien, Institute of Lightweight Design and Structural Biomechanics), H. Pettermann (TU Wien, Institute of Lightweight Design and Structural Biomechanics)

Shell-based ply-level (SPL) models are a computationally efficient approach to separately treat intra-ply damage and delamination in finite element simulations of layered composite structures. However, conventional SPL models cannot capture the out-of-plane stresses correctly and also the elastic deformations with respect to transverse shear loading are strongly underestimated for thick composites. This is an implication of the plane-stress assumption of the shell elements and the infinitely thin and quasi-rigid cohesive zone elements (CZE) used to model the interfaces between adjacent plies.
The issues of conventional SPL models can be overcome by assigning the CZE a subset of the 3D continuum behavior comprising the out-of-plane properties of the adjacent plies and the properties of the interface between the plies. The applicability of the extended SPL model is verified by using the example of a thick layered composite plate subjected to transverse shear loading where different composite lay-ups are considered. As reference a corresponding models with continuum element discretization are used. The transverse shear stresses and deformations estimated by the extended SPL models are in perfect agreement with the results of the continuum model. In most cases the errors are below 1%. Furthermore, the membrane stresses in the shells are not compromised and perfectly resemble the continuum solution. Only for composite lay-ups which show a strong bending-to-twisting coupling slightly larger differences occur for the deformations (approx. 3%), whereas the stresses can still be well predicted.
Concluding it can be said, that for the modeling of layered composite structures the extended SPL approach provides high reliability of the results in combination with high computational efficiency.

Stress-based mixed finite elements for elasticity

F. Bertrand (University of Duisburg-Essen), G. Starke (Universität Duisburg-Essen), M. Moldenhauer (Universität Duisburg-Essen)

Computations in solid mechanics are usually performed using the displacements as primal variable. As accurate stress approximations are of interest in many applications in solid mechanics, their reconstruction has to be produced carefully. In particular, reconstruction algorithms should be localizable and obey certain local average momentum balance properties.
An alternative approach consists in the use of variational formulations involving the stress as an independent variable which is approximated directly in suitable $H(div)$-conforming finite element spaces. The standard mixed finite element (see e.g. [3]) approach leads then to a saddle-point problem, in which the momentum balance is approximated in an optimal way, if appropriate finite element combinations are used. However, the construction of those finite element spaces is challenging, since a stability

condition between the mixed spaces has to be established.
In order to avoid the complexity of this stability condition, a positive definite system can be obtained by minimizing the residuals in the partial differential equations. Using the L^2-norm leads to the Least-Squares method (see e.g. [1]), which provides the advantage of an inherent a posteriori error estimator. Due to the strong connection of this stress approximation to that obtained from a mixed formulation, the error associated with the momentum balance can be proved to be of higher order than the overall error of the least-squares approach. This implies that the favorable conservation properties of the dual-based mixed methods and the error control of the least squares method can be combined.
On domains with curved boundaries, stress approximations in Raviart-Thomas needs to be produced in the parametric Raviart-Thomas spaces studied in [2]. The use of this framework and of the actual configuration allows to extend the linear models to the nonlinear case for hyperelastic material, involving geometrical and material nonlinearities. This leads to a nonlinear mixed formulation with linear constraint, in which the symmetry of the stress tensor can be preserved.

1. 1 F. Bertrand, S. Münzenmaier, and G. Starke, *First-Order System Least Squares on Curved Boundaries: Higher-order Raviart-Thomas Elements.* SIAM J. Numer. Anal. 52.6 (2014): 3165-3180.

2. 2 P. Bochev and M. Gunzburger, *Least-Squares Finite Element Methods*, Springer, New York, 2009.

3. 3 D. Boffi, F. Brezzi, and M. Fortin, *Mixed Finite Element Methods and Applications.* Springer-Verlag, Heidelberg, 2013.

Structure-Preserving Optimal Control for Mechanical Systems

K. Flaßkamp (Universität Bremen), C. Büskens (Universität Bremen)

Optimal control tasks as they arise in robotics, biomechanics, or automotive engineering, can be challenging to solve due to nonlinear models which require high-dimensional discretizations and a high number of (nonlinear) constraints. Direct optimal control methods transcribe the problem into an optimization problem so that fast NLP solvers can be applied. This can be complemented by transcription techniques that allow for efficient algorithm design. The poster presents research in performing this discretization by variational integrators for mechanical systems. This approach allows to preserve structures on two levels: firstly, those of the (continuous-time) dynamical system and secondly, the Hamiltonian structure of the optimal control problem. We further show recent applications of optimal control with variational integrators.

Economic model predictive control

M. Müller (University of Stuttgart)

Model predictive control (MPC) is a control technique which consists of repeatedly solving a finite horizon optimal control problem and then applying the first part of the solution to the considered system. The main advantages of MPC and the reasons for its widespread success in many applications are that (i) satisfaction of hard input and state constraints for the closed-loop system can be guaranteed, (ii) optimization of some performance criterion is directly incorporated in the controller design, and (iii) it can be applied to nonlinear systems with possibly multiple inputs. Most MPC results in the literature consider the classical control objective of setpoint stabilization; to this end, the stage cost function in the optimal control problem is chosen to be positive definite with respect to this setpoint. On the other hand, the main focus in *economic* MPC lies on the optimization of some general performance criterion, which needs not be related to any specific steady-state to be stabilized. These type of control problems arise in many different fields of application, including, e.g., the process industry, building climate control, or the control of wind turbines.
A distinctive feature of economic MPC is the fact that the closed-loop trajectories do not necessarily converge to a steady-state, but can exhibit more complex, e.g., periodic, behavior. In particular, the optimal operating behavior for a given system depends on its dynamics, the considered performance criterion and the constraints which need to be satisfied. In this poster presentation, we discuss characterizations of different optimal operating behaviors by means of dissipativity. In particular, we show that under rather mild controllability conditions, both optimal steady-state operation and optimal periodic operation can equivalently be characterized by suitable dissipativity conditions, see [1, 2]. Moreover, we discuss how suitable economic MPC schemes can be designed in case that uncertainties and disturbances are present. Compared to stabilizing MPC schemes, new methods how to counteract disturbances have to be developed in order to achieve good closed-loop performance. We present different robust and stochastic economic MPC approaches which are suitable under different assumptions on the disturbances and discuss the achievable performance guarantees [3, 5].

[1] M. A. Müller, D. Angeli, and F. Allgöwer. On necessity and robustness of dissipativity in economic model predictive control. IEEE Transactions on Automatic Control, vol. 60, no. 6, pp. 1671-1676, 2015.

[2] M. A. Müller, L. Grüne, and F. Allgöwer. On the role of dissipativity in economic model predictive control. In Proc. of the 5th IFAC Conference on Nonlinear Model Predictive Control, Seville, Spain, 2015, pp.110-116.

[3] F. A. Bayer, M. Lorenzen, M. A. Müller and F. Allgöwer. Robust economic model predictive control using stochastic information. Automatica, vol. 74, pp. 151-161, 2016.

[4] F. A. Bayer, M. A. Müller, and F. Allgöwer. Min-max economic model predictive control approaches with guaranteed performance. In Proc. of the 55th IEEE Conference on Decision and Control (CDC), Las Vegas, USA, 2016.

Edge, Ridge and Blob Detection With Symmetric Molecules

R. Reisenhofer (Universität Bremen), E. King (Universität Bremen)

We present a novel approach to feature detection, in which the symmetry properties of directionally sensitive analyzing functions constructed in the so-called α-molecule framework can be exploited to detect edges, ridges and blobs in images. Furthermore, we show how additional information, such as the widths of ridges and blobs or local tangent orientations of edges and ridges can be extracted by analyzing the behavior of coefficients corresponding to differently scaled and oriented symmetric molecules.

For each type of feature, a measure is defined that assigns values ranging from 0 to 1 to each point in an image denoting the likelihood that an edge, ridge or blob is centered at the respective location. These measures are based on inner products of the considered image with differently scaled and oriented α-molecules generated by applying rotation and scaling operators to even- and odd-symmetric generating functions. The measures are by construction contrast invariant, stable in the presence of noise and capable of detecting features arising both from smooth and sharp transitions.

Reduced order homogenization for nonlinear composite materials with imperfect interfaces at the phase boundaries

M. Leuschner (University of Stuttgart), F. Fritzen (Universität Stuttgart)

Numerical homogenization schemes for nonlinear composite materials are often related to enormous computational cost, which is prohibitive for realistic three-dimensional multiscale simulations. The high number of executions of the homogenization routine in such simulations easily justifies the effort required for the time-consuming training of a reduced order model.
The potential-based Reduced Basis Model Order Reduction (pRBMOR) homogenization technique is an example of such a reduced order method. One of its key ideas is to introduce reduced bases for the fields of microscale internal variables. Another important aspect is the utilization of potential-based microscale constitutive models from the class of Generalized Standard Materials (GSM). GSM models have a variational structure which is transferred to the macroscale. In combination with the reduced basis ansatz, the macroscale variational problem can be solved in an efficient algorithm without costly iterations at the microscale.
By introducing a reduced basis for the field of displacement jumps at the phase boundaries, the pRBMOR technique has recently been applied to microstructures with imperfect interfaces. The main ideas of the pRBMOR extended in this manner will be presented. Further, an example combining viscoplasticity in the matrix material with viscoelastic interfaces is shown.

Error Estimation in Multiphysics Problems using Runge Kutta Methods with Additive Partitioning

U. Römer (Technische Universität Darmstadt), A. Sandu (Virginia Polytechnic Institute and State University)

This work addresses problems driven by multiple physical processes which may evolve on multiple scales. For this class of problems, dedicated solvers can be obtained within the framework of generalized additive Runge-Kutta methods (GARK) [1]. In multiphysics applications, numerical approximation errors can interact in a complex way. Hence, for the accuracy and efficiency of a numerical method these errors need to be estimated and controlled. To this end, we use the discrete adjoint approach. We show, that under certain restrictions on the weights, the adjoint problem can also be formulated as a GARK method and analyze the propagation of errors in the different sub-problems. Numerical results for a reaction-diffusion problem are given to illustrate the findings.

[1] Adrian Sandu, and Michael Günther, A Generalized-Structure Approach to Additive Runge–Kutta Methods, *SIAM Journal on Numerical Analysis*, vol. 53, 2015, pp. 17–42.

Rank-one convexity implies polyconvexity for isotropic energies on SL(2)

I. Ghiba (Alexandru Ioan Cuza University of Iași), R. Martin (University of Duisburg-Essen), P. Neff (University of Duisburg-Essen)

We study convexity properties of energy functions in plane nonlinear elasticity of incompressible materials and show that rank-one convexity of an objective and isotropic elastic energy W on the special linear group SL(2) implies the polyconvexity of W.

Stress-Based and Strain-Based Blood Damage Estimation for Medical Device Design

L. Pauli (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), M. Behr (RWTH Aachen University, Chair for Computational Analysis of Technical Systems)

The development of reliable blood damage models is a key issue for the virtual design of ventricular assist devices (VADs). VADs are used to provide mechanical circulatory support to chronically ill heart disease patients. The mechanical hemolysis in VADs is an example for a microscale effect that can only be measured on the macroscale. Therefore, hemolysis is usually modeled as a bulk phenomenon and based on a simple power law, depending on scalar shear-stress and exposure time. In the commonly used stress-based model, the scalar shear stress depends solely on the precomputed Navier-Stokes equations. The stress-based model is only able to account for macroscale phenomena and therefore, it implicitly assumes that red blood cells (RBCs) deform instantaneously. A different approach is a simulation by means of a strain-based model. Here, the viscoelastic deformation of RBCs is computed by a tensorial evolution equation. The tensor results are used to estimate a distortion of RBCs in the flow field. With the distortion, an effective shear stress can be computed, which is acting on the RBC itself [1]. As a

consequence, microscale effects are considered in the simulation, even though the overall result is on the macroscale.
The flow field and hemolysis quantities in VADs are computed by stabilized space-time finite element methods. The impeller movement in VADs is incorporated by either a multiple reference frames method [3], or a moving mesh technique based on the ALE formulation and the shear-slip mesh update method. Turbulence is considered by large eddy simulation. Hemolysis is computed by an Eulerian or field-based approach. The Eulerian approach allows simple identification of critical regions in the pump, which is useful for computer-aided design optimization.
Comparisons of stress-based and strain-based hemolysis models in a benchmark blood pump show very significant differences. Stress peaks with short exposure time contribute to the overall hemolysis in the stress-based model, whereas regions with increased shear and long exposure time are responsible for damage in the strain-based model [3].

[1] L. Pauli, J. Nam, M. Pasquali, and M. Behr. Transient Stress-Based and Strain-Based Hemolysis Estimation in a Simplified Blood Pump. *International Journal for Numerical Methods in Biomedical Engineering*, 29(10):1148–1170, 2013.

[2] L. Pauli, J.W. Both, and M. Behr. Stabilized finite element method for flows with multiple reference frames. *International Journal for Numerical Methods in Fluids*, 78:657–669, 2015.

[3] L. Gesenhues, L. Pauli, and M. Behr. Strain-Based Blood Damage Estimation for Computational Design of Ventricular Assist Devices. *The International Journal of Artificial Organs*, 39(4):166–170, 2016.

Feature Selection From Real-World Data With Non-Linear Observations

M. Genzel (TU Berlin), G. Kutyniok (TU Berlin)

A fundamental challenge in machine learning is the *selection of discriminative features* from a relatively small collection of sample pairs $\{(x_i, y_i)\}_{1\leq i\leq m}$. Here, the *observations* $y_i \in \mathbb{R}$ are often supposed to follow a noisy single-index model, depending on a certain set of *target variables*. The major difficulty is now that these variables cannot be observed directly, but rather arise as *hidden* factors in the actual *data vector* $x_i \in \mathbb{R}^d$ (*feature variables*). A typical example would be *mass spectrometry data* of the human proteome, where the desired molecular concentrations of proteins are intrinsically encoded by means of Gaussian-shaped peaks.
In this presentation, we will see that a successful feature selection is still possible when the applied estimator does not have any knowledge of the underlying data representation and only takes the "raw" samples $\{(x_i, y_i)\}_{1\leq i\leq m}$ as input. Guarantees of such type are especially appealing for practical purposes, since in many applications even standard methods, e.g., the Lasso or logistic regression, yield surprisingly good outcomes. The mathematical basis of our results forms a recent framework for structured signal recovery from highly underdetermined (non-)linear equation systems. This allows us to

treat the problem of feature selection in a unified way, particularly including *non-linear observations*, arbitrary *convex signal structures* as well as *strictly convex loss functions*. This is joint work with Gitta Kutyniok.

A polyconvex phase-field approach to fracture with application to finite-deformation contact problems

M. Franke (Karlsruhe Institute of Technology), M. Dittmann (University of Siegen), C. Hesch (University of Siegen), P. Betsch (Karlsruhe Institute of Technology)

Variationally consistent phase-field methods are able to efficiently simulate complex three-dimensional fracture problems (see [1, 2]). However, the developments for large deformations often exhibit a lack of numerical stability for different loading scenarios. In this talk we present a novel formulation for finite strain polyconvex elasticity by introducing a new anisotropic split based on the principal invariants of the right Cauchy-Green strain tensor which ensures polyconvexity of the resulting strain energy function (see [4]). Furthermore the variationally consistent Mortar contact algorithm is applied (see [3]) to handle complex contact boundaries. In order to improve accuracy a fourth order Cahn-Hilliard crack density functional is used. To account for the C^1 requirement the system is embedded in a sophisticated isogeometric framework with local refinement. The new polyconvex phase-field fracture formulation guarantees numerical stability for arbitrary hyperelastic materials. The performance of the proposed methods will be examined in representative numerical examples.

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Approximation of Generalized Ridge Functions in High Dimensions

S. Keiper (TU Berlin)

The approximation of functions in many variables suffers from the so-called "curse of dimensionality". Namely, functions on $\mathbb{R}^N$ with smoothness of order s can in general be recovered at most with an accuracy of $n^{-s/N}$, applying n-dimensional spaces for linear or nonlinear approximation. To impose more structure on f, different models have been considered. One of the most popular is that of so-called ridge functions, which are constant along certain linear subspaces. However, assuming that real world problems can be described by such functions is very restrictive. Therefore, we want to present an analysis of generalized ridge functions, namely of functions which are constant along certain submanifolds of $\mathbb{R}^N$. For this, we will introduce the notion of sleeve functions. We will then investigate and analyze algorithms for the approximation of so-called linear-sleeve functions and propose an approach of how to apply these algorithms to capture general sleeve functions.

6 Sections

S 1: Multi-body dynamics

Organizers: Jörg Fehr (Institute of Engineering and Computational Mechanics, University of Stuttgart)
Jürgen Pannek

S 1 : Multi-body dynamics

Tuesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 105

Challenges in Modeling Flexible Bodies based on Experimental Data with Utilization in Elastic Multibody Simulation

C. Lein (TU Dresden, Fakultät Maschinenwesen), J. Woller (TU Dresden, Fakultät Maschinenwesen), M. Beitelschmidt (TU Dresden, Fakultät Maschinenwesen) 14:00

The Elastic Multi-Body Simulation (EMBS) progressively constitutes the established method when dealing with elastic deformations of components in complex mechanical systems. The Floating-Frame-of-Reference-Formulation (FFRF) is the state-of-the-art method, whereas the model of the elastic body is usually generated by the Finite-Element-Method (FEM). However, the FE-model consists of several uncertainties concerning geometry, mass distribution, local and directional stiffness as well as damping phenomena. For representing realistic components, in many cases an expensive model-updating based on measured data is necessary. A Model Order Reduction (MOR) is the next step in the conventional process condensing the elastic degrees of freedom, which embodies further approximation errors. Finally, the information of the elastic body model is passed to the EMBS using the Standard Input Data (SID) file format.
Due to the complex and error-prone conventional procedure, a novel approach is suggested, where the data of the elastic body model is directly gained from the results of an Experimental Modal Analysis (EMA) without using any FE-model or MOR. This novel approach yields five challenges that need to be dealt with: A proper measurement setup (free-free support and measurement points), the parameter identification (extraction of modal information), a correct representation of the mass distribution, the treatment of rotational coordinates and the creation of interface nodes for the EMBS-couplings.
The contribution presents solutions for the mentioned challenges and shows results of the novel approach using an U-section as validation example. The whole procedure is performed for the MBS-software SIMPACK version 9. The processing of the experimental data and generation of the SID are realized by means of the software MORPACK

(Model Order Reduction PACKage), which is developed at the chair of dynamics and mechanism design.

Higher-Order Index-1 Co-Simulation Approach: Solver Coupling for Multibody Systems

T. Meyer (TU Darmstadt), B. Schweizer (TU Darmstadt), P. Li (TU Darmstadt), D. Lu (TU Darmstadt) 14:20

This contribution attends to a co-simulation approach for solver coupling in time domain. A general multibody system is divided into several subsystems, which are coupled by algebraic constraint equations. The coupling technique analyzed here is a linear-implicit predictor/corrector approach, i.e. coupling variables for the corrector step are calculated by one step of a *Newton*-iteration. At the communication-time points the coupling conditions together with its first and second derivatives are satisfied simultaneously, except for the error of the *Newton*-iteration. This index-1 approach uses cubic polynomials to approximate the coupling variables. The space of polynomials of degree ≤ 3 is a four-dimensional vector space. One of the four degrees of freedom is used for a continuous approximation of the coupling variables at the communication-time points. The three remaining degrees of freedom are used in order to enforce the coupling equations on position, velocity, and acceleration level. Due to the higher order approximation, the numerical errors are very small and a good convergence behavior is achieved.

[1] Arnold, M.: Stability of sequential modular time integration methods for coupled multibody system models. J. Comput. Nonlinear Dyn. 5, 1–9 (2010)

[2] Schweizer, Bernhard, and Daixing Lu. "Stabilized index-2 co-simulation approach for solver coupling with algebraic constraints." Multibody System Dynamics 34.2 (2015): 129–161, doi:10.1007/s11044-014-9422-y.

[3] Schweizer, Bernhard, Pu Li, and Daixing Lu. "Implicit co-simulation methods: Stability and convergence analysis for solver coupling approaches with algebraic constraints." ZAMM–Journal of Applied Mathematics and Mechanics (2015), DOI: 10.1002/zamm.201400087.

Simulation of the dynamics of flexible mounted machines with nonlinear spring elements

E. Gerlach (TU Ilmenau), B. Fiedler (TU Ilmenau) 14:40

This contribution presents ideas, how influence undesired interactions between ground and machines, e.g., vibrations. While designing machines hook up, it is often important to minimize the dynamic load on the ground. One possibility is the optimal design of the stiffness and damping properties of the elastic mountings to reduce the emission of vibrations [1]. For this purpose, rubber elements, metal cushions, hydraulic bearings or form springs are often used. But to design these components well, an accurate knowledge of the excitation is required. If there are no or only few information about the excitation,

numeric simulations could be performed to analyze different scenarios. The multi-body simulation software ALASKA is used to analyze a simplified model of the system (e.g. centrifuge). The model consists of rigid bodies and the elastic support. The elastic support is represented by a combination of commonly used elements incorporated in ALASKA. They form a series circuit. Element one is a spring/damper element with nonlinear properties, it is modelling within the limits of the Kevin-Voigt model. Model parameter are measured by a real rubber element. The second element is characterized by the behavior of a nonlinear form spring.
The dynamic behavior of the mechanical system could be described by a system of differential equations of the form:

$$M\ddot{\vec{q}} + K\dot{\vec{q}} + C\vec{q} = \vec{Q}$$

The elements of the matrices M, K and C are constant or variable in time. Matrices K and C depend on the elastic support. Changing the coefficients and the loading different simulations are done to study the system behavior.

[1] H.Dresig, F.Holzweißig: Maschinendynamik, 12. Auflage, Springer, Berlin, Heidelberg, 2016

Effective preconditioning techniques for domain decomposition methods for nonlinear dynamic systems arising in multibody dynamics

E. Dewes (Lehrstuhl für Angewandte Mechanik, TU München), D. Rixen (Lehrstuhl für Angewandte Mechanik, TU München) 15:00

Domain decomposition methods, in particular the finite element tearing and interconnecting (FETI) method, have proven to be highly efficient in solving large-scale finite element problems arising in structural dynamics. Their good numerical and parallel scalability is also promising for application to flexible multibody system dynamics.
In many engineering applications, one can assume that the deformations within each flexible body are small, but the overall motion is non-linear and described typically by a co-rotated floating frame. The challenge is then to solve the overall non-linear system efficiently with domain decomposition techniques, which seems a natural approach since each body can be considered as a domain. Especially non-constant jacobians originating from nonlinear constraint equations require good preconditioning techniques to keep computational costs low and preserve scalability.
In this contribution, in order to simulate the dynamic behaviour of constrained multibody systems, we present a time integration scheme, which is based on a generalized-α method with an embedded FETI method to solve the linear systems arising in every time step within the Newton iterations. We investigate different types of FETI-preconditioners in the context of multibody system dynamics concerning perfomance, numerical stability and scalability. We validate our results numerically based on an academical test model.

[1] Arnold, Martin ; Brüls, Olivier: Convergence of the generalized-α scheme for constrained mechanical systems. In: *Multibody System Dynamics* 18 (2007), Nr. 2, 185–202. http://dx.doi.org/10.1007/s11044-007-9084-0. – DOI 10.1007/s11044–007–9084–0. – ISSN 1573–272X

[2] Farhat, Charbel ; Roux, Francois-Xavier: A method of Finite Element Tearing and Interconnecting and its parallel solution algorithm. In: *International Journal for Numerical Methods in Engineering* 32 (1991), S. 1205–1227

[3] Rixen, Daniel J.: Extended preconditioners for the FETI method applied to constrained problems. In: *International Journal for Numerical Methods in Engineering* 54 (2002), Nr. 1, 1–26. http://dx.doi.org/10.1002/nme.412. – DOI 10.1002/nme.412. – ISSN 1097–0207

Interface-Reduction for Substructured Mechanical Systems with Constraints Using General Singular Value Decomposition

N. Walker (University of Stuttgart), P. Eberhard (University of Stuttgart) 15:20

During the development of new products, different components are usually designed separately. Therefore, a modular setup of simulation models, as provided in substructured finite-element models or in flexible multibody systems, is advantageous. If the finite-element models of the components are densely meshed, the simulation might get expensive. Therefore, a model order reduction is performed. In substructured settings, model order reduction including moment matching has shown to be advantageous. One major drawback of these methods is that the minimal order of the reduced model depends directly on the number of interactions. Especially when structures are coupled via surfaces, this might be a decisive restriction. This motivates the use of interface-reduction methods on such surfaces. The coupling between the bodies can be modeled via force elements or via constraints. For coupled systems with bushings, interface-reduction using General Singular Value Decomposition (GSVD) has shown good approximation quality. However, the use of the method for bodies coupled via constraints is not straight forward. In this contribution an approach for interface reduction using GSVD for substructured mechanical systems with constraints is presented and compared to other interface-reduction methods.

The Boundary Layer Machine

G. Ostermeyer (TU Braunschweig), T. Vietor (TU Braunschweig), M. Müller (TU Braunschweig), D. Inkermann (TU Braunschweig), J. Otto (TU Braunschweig), H. Lembeck (TU Braunschweig) 15:40

In multi-body systems, friction often occurs as a result of the contact between two bodies. These forces may be desirable or undesirable, depending on the intended function of a technical system. Although many conceivable causes of these forces have been described, the scientific understanding of friction is still incomplete.

A new, holistic approach is to be taken, in order to recognize and describe the general design principles of friction contacts. These principles may also be employed towards the formulation of design guidelines. When two bodies are in contact, many additional effects can be observed along with friction. From a holistic viewpoint, the design of "two bodies in contact" can be understood as a highly complex machine. The capabilities of this machine include, but are not limited to:
- generation of forces,
- generation of heat,
- generation of elastic and acoustic waves including ultrasonic waves,
- generation of wear particles,
- generation of material transport with various forms of self-organization,
- generation of surface changes on highly differing scale sizes, and
- generation of chemical reactions.
These effects are all dynamically coupled with one another. The boundary layer machine represents the simplest possible "machine" in a multi-body system.

S 1 : Multi-body dynamics

Tuesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 105

The long History of Impact Mechanics, Rolling Contact and Multibody System Dynamics

W. Schiehlen (University of Stuttgart) 16:30

Contact mechanics is a branch of solid mechanics where two or more bodies are involved. The contacting points are characterized by a common tangential plane and a common normal vector given by the surface curvature of the bodies. Additional parameters of contact problems are the material of the bodies, the forces and torques acting on the bodies as well as their time history, location of the centers of mass and the roughness of the surface around the contact point. The classical contact problem solved by Hertz (1882) is based on spherical bodies surfaces, linear-elastic material, constant static loading in normal direction and smooth surfaces. The rigorous results are often used as benchmarks. Details can be found in the monographs of Johnson (2003) and Popov (2015). The bodies of mechanical systems in engineering applications get in contact to each other mainly by impacts, rolling or sliding, or by joints.
Impacts of bodies by collisions result in strongly augmented forces what is known to humans since ancient times. The first human tools have been originally hand-axes made of rock which were replaced by hammers about 10 thousand years ago. Today, hammers are used by everybody. They are now properly designed with shaft lengths considering the center of impact to avoid reaction forces in the worker's hand. In antiquity already the philosopher Aristotle stated the question on the augmentation of impact forces, he

imagined a lever action. In the Middle Ages many scientists started working on impact problems as reviewed by Szabo (1977). The recent state of the art was presented by Sändig, Schiehlen and Wendland (2000).
Rolling contact plays a unique, central and dominant role for human mobility. The two contacting bodies involved are the wheel and the guideway. And these two parts are not available in our natural environment, they were invented by humans. Most of the other kinds of transportation like flying, swimming or diving have been inspired by birds and fishes. This is the reason why the wheel was invented very recently, namely 3.500 years before Christ. For comparison, the life on our planet started 4 billion years ago. The first rail tracks were laid 1767 in UK for horse drawn vehicles and since 1825 for railways. The first asphalt roads were built around 1850 in France, and in 1885 the first car powered by a gasoline engine was successfully completed by Benz in Germany. This means that by the end of the 19th century the basic components for the mechanization of transport were invented. The rolling contact, Carter (1926) and Kalker (1967) or Pacejka (1975), respectively, considered linear or nonlinear material, cylindrical wheel disks and planar guideways, rough surface with friction, static loading and steady-state rotating wheels. For details see Popp and Schiehlen (2010).
Multibody System Dynamics provides engineering software tools for design, simulation and testing of complex dynamical systems, too, in particular for vehicle systems. The fundamental equations are based on classical mechanics. Newton published his three laws in 1686 while Euler added his equations in 1775. During the late Middle Ages many dynamics principles were published, see Szabo (1977). A major progress was achieved by the availability of digital computers half a century ago. Two more recent review papers by Schiehlen (1997) and Shabana (1997) deal with multibody dynamics. Thus, not only the analytical beauty but also the computational efficiency of the algorithms is now important for modelling and visualization of vehicle systems. The contact between the bodies by joints is in multibody system codes as a standard implemented but the wheel-guideway forces of the rolling contact have to be added to complete the vehicle system as discussed in this session on multibody dynamics.

[1] Carter, F.W.: On the action of a locomotive driving wheel. Proc. Roy. Soc. A; 112-151 (1926)

[2] Hertz, H.: Über die Berührung fester elastischer Körper (in German). Journal reine angewandte Mathe. 92, 156 - 171 (1882)

[3] Johnson, K.L.: Contact Mechanics. Cambridge University Press, Cambridge (2003)

[4] Kalker, J.J.: On the Rolling Contact of Two Elastic Bodies in the Presence of Dry Friction. PhD Thesis, TH Delft (1967)

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[6] Popov, V.: Kontaktmechanik und Reibung (in German). Springer (2015)

[7] Popp, K. and Schiehlen, W.: Ground Vehicle Dynamics. Springer (2010)

[8] Sändig, A.M.; Schiehlen, W. and Wendland, W.L.: Multifield Problems – State of the Art. Springer, Berlin 2000.

[9] Schiehlen, W.: Multibody System Dynamics: Roots and Perspectives. Multibody System Dynamics 1, 149 – 188 (1997)

[10] Shabana, A.A.: Flexible Multibody Dynamics: Review of Past and Recent Developments. Multibody System Dynamics 1, 189 – 222 (1997)

[11] Szabo, I.: Geschichte der mechanischen Prinzipien (in German). Birkhaeuser, Basel (1977)

Vehicle Modeling by non-perfect Multi-body Systems

G. Rill (OTH Regensburg), T. Schaeffer 16:50

Virtual prototyping has become a common tool in the automotive industry. Commercial software packages make it possible to set up sophisticated and complex three-dimensional vehicle models. Some providers even offer complete vehicle models with a comfortable graphical user interface. However, sophisticated vehicle models are not only required in the automotive industry and their suppliers but also in the academic research community that develops new control strategies in order to improve the comfort and ride safety of vehicles. To avoid costly licence fees, rather simple models, generated by the specific researcher, are commonly used for that purpose. However, a modeling technique tailored to the specific properties of vehicles makes it possible to set up fully non-linear and three-dimensional vehicle models with reasonable effort. This models require a minimum number of floating point operations and will run in real-time even on small computers. The paper shows, that Jourdain's principle combined with non-trivial generalized velocities results in a straight forward and rather simple procedure for generating the equations of motion for road vehicles. In addition, some acceleration terms that are very cumbersome to calculate, may be neglected due to the specific properties of vehicle suspension systems. Simulation results illustrate that the resulting non-perfect multi-body vehicle system is valid in all operating conditions.

Configuration spaces with Lie group structure: A novel approach and its application to a Cosserat beam model

S. Hante (Martin-Luther-Universität Halle-Wittenberg), M. Arnold (Martin-Luther-Universität Halle-Wittenberg) 17:10

In multibody dynamics, the parametrization of the bodies' configuration plays a crucial role. Large rotations often appear and thus have to be described in a way that is free from singularities. Popular parametrizations are $SO(3)$ and unit quaternions $\mathbb{S}^3$.
We present the semi-direct product $\mathbb{S}^3 \ltimes \mathbb{R}^3$ as a novel approach to configuration spaces of rigid bodies and the relation to and advantages over established configuration spaces such as $SE(3)$ or dual quaternions.

Subsequently, we present a Cosserat beam model, where the beam is parametrized by a time-dependent curve in $\mathbb{S}^3 \ltimes \mathbb{R}^3$. We show the advantages over parametrizations involving the direct product $\mathbb{S}^3 \times \mathbb{R}^3$. While the equations of motion may be obtained by a two-dimensional variational principle (Lang, Linn 2009), we use a discretized variational principle in order to obtain semidiscrete equations of motion, thus applying a method of lines. The resulting equations can be interpreted as the equations of motion of n rigid bodies and therefore a differential equation of second order on the Lie group $\left(\mathbb{S}^3 \ltimes \mathbb{R}^3\right)^n$. We show results, where a generalized-α Lie group time integrator was applied for time integration.

S 1 : Multi-body dynamics

Wednesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 105

Dynamical Analysis of a Tip Balancing Cube

H. Gattringer (Johannes Kepler University Linz), A. Reiter, C. Stöger (Johannes Kepler University Linz), M. Jörgl, A. Müller (Johannes Kepler University Linz) 14:00

The paper discusses some dynamical aspects of a self-balancing Inertia Wheel Cube (IWC). The acceleration and deceleration of actuated flywheels is used to stabilize the IWC balancing on one of its corners, which is an unstable equilibrium position. The orientations as well as the rotational velocity of the device are measured by an inertial measurement unit (IMU). The equations of motions are derived with the Projection Equation. Using the rotational velocity of the IWC as part of the generalized velocities leads to well-structured and interpretable dynamical equations. These equations are the basis for simulation, parameter identification, control synthesis, and stability analysis. The stability of the unstable equilibrium is investigated by means of the linearized motion equations. It turns out that there are always uncontrollable states due to the conservation of momentum. A further analysis considers offsets in the orientation measurement with the IMU and the imprecisely knowledge of the center of gravity. These offsets lead to constant flywheel speeds for the PD controlled IWC. In order to compensate this negative effect an observer for the center of gravity is introduced. Simulations as well as experimental results are presented.

A robot inspired by a non-smooth point mass model of a worm

T. Winandy (University of Stuttgart), S. Eugster (University of Stuttgart) 14:20

An earthworm travels using waves of muscular contractions which alternately shorten and lengthen the body. The skin of the earthworm carries claw-like bristles, which anchor the shortened part of the body to the soil.

We present a planar model of a chain of five point masses that mimics the worm-like locomotion. The point masses are aligned horizontally on the ground. The muscles of

the worm are modelled by including a force law between each pair of neighbouring point masses. The four force laws allow the actuation of the chain. The choice of the force laws allows to consider different types of actuators and to compare various actuation patterns. The contacts of the elements with the ground are idealized as being unilateral constraints subjected to friction. It is the inclusion of friction, which enables the chain to advance on the ground. The influence of the worm's claw-like bristles can be investigated by considering anisotropic friction. Inspired by the promising results of the numerical model, a prototype has been designed. It consists of five rigid blocks and is actuated by four solenoids.

Structural Synthesis of Parallel Robots with Unguided Linear Actuators

S. Schulz (Hamburg University of Technology), A. Seibel (Hamburg University of Technology), J. Schlattmann (Hamburg University of Technology) 14:40

Although there are plenty of other methods and formulae, the Chebychev-Grübler-Kutzbach (CGK) formula and the extended CGK formula are most widely used to calculate the degree of freedom (DOF) of serial as well as parallel mechanisms. Gogu proved (Gogu 2008) on the example of a specially developed mechanism that, up to now, no method or formula is able to fit for all mechanisms. Especially for parallel mechanisms, the existing methods and formulae that are used to calculate the mechanism's mobility shall be handled carefully.

Consider a parallel structure with six identical chains of variable length, for example, the Gough-Stewart Platform. There exist two similar types, the 6-UPS and the 6-SPS type. Here, U stands for 'universal', P for 'prismatic', and S for 'spherical'. The 6-UPS parallel robot has six DOF and no redundancy, while the 6-SPS parallel robot has also six DOF but six degrees of redundancy (Gogu 2008). Usually, prismatic joints (P joints) are considered with one DOF. This is equivalent to a guided linear actuator because there is no rotation possible between the upper and the lower part of the linear actuator. Unguided linear actuators, for example, ball screw linear actuators or hydraulic driven linear actuators with a piston rod, are not similar to prismatic joints, and therefore, they cannot be completely described by a prismatic joint. Hydraulic driven linear actuators with an unguided piston rod must be taken into account as a series connection of a prismatic joint and a revolute joint (R joint).

Now, consider a Gough-Stewart Platform with unguided linear actuators, in this case, ball screw linear actuators. In this paper, we show that this parallel robot has to be described by a series connection of a helical joint (H joint) and a revolute joint (R joint) and has six DOF in the actuated operation state and less than six DOF in the non-operation state. The change of the length that results from the passive rotation between the lower and the upper cylinder of the linear actuator, which must not be confused with the passive rotation of the platform due to the universal joints (Du et al. 2016), has to be compensated actively. For this reason, it is sufficient to use universal joints instead of spherical joints which results on one hand in an accurate and redundancy-free motion and on the other hand in a lager work-space and lower costs. The parallel robot can

then be described by a 6-UHRU type.

S. Gogu.: *Structural Synthesis of Parallel Robots, Part 1 – Methodology.* Springer-Verlag, Dordrecht, Netherlands, 2008.
Du, S.; Schlattmann, J.; Schulz, S.; Seibel, A.: *Passive Rotation Compensation in Parallel Kinematics using Quaternions.* In: *Proceedings in Applied Mathematics and Mechanics* 16(1): 51−52, 2016.

Vibration Damping of Flexible Link Robots Using an Eye-in-Hand Camera

F. Pucher (Johannes Kepler University Linz), H. Gattringer (Johannes Kepler University Linz), A. Müller (Johannes Kepler University Linz) 15:00

Robots with flexible links are used in fields where high dynamic requirements have to be fulfilled. Since the main goal of the control is to achieve a precise positioning, the damping of oscillations due to the low stiffness is imperative. For simulation and control design a dynamic model of the robot is necessary. Aiming at computationally efficient models, the elastic deformations are modeled by springs coupling the motor shaft with a rigid robot arm. The equations of motion are calculated by using the Projection Equation in subsystem representation. The model of an elastic robot is uncontrollable when only measurements of the motor motions are available. Therefore, acceleration sensors are usually attached at the robot's end-effector to provide sufficient measurements. Further a pure PD control is insufficient for vibration damping. This paper presents an approach using an Eye-in-Hand camera for vibration damping of an elastic articulated robot with three actuated joints. The idea is to use the position of feature points in the camera image for generating a feedback signal. Three circular markers are detected via image processing. The grayscale image is converted into a binary image where the marker contours are found. Due to parallel projection a circle is displayed as an ellipse that is fitted to approximate the contour points. With the inverse kinematics the image feature position error is mapped to the error of the arm angle by using the image-Jacobian. The PD-motor joint control is augmented by a proportional term w.r.t. the arm angle. Finally the experimental results of a comparison with a control concept based on acceleration sensors are presented.

Parameter Identification of Non-Holonomic, Omnidirectional Vehicles using a Redundantly Parameterized Model

C. Stöger (Johannes Kepler University Linz), A. Müller (Johannes Kepler University Linz), H. Gattringer (Johannes Kepler University Linz) 15:20

Non-holonomic, omnidirectional vehicles have a high maneuverability and payload capacity but suffer from kinematic singularities. The usage of redundant coordinates allows to describe the systems dynamics without the need to switch between different sets of generalized coordinates. This paper presents a method for identifying the parameters of such a system. The method enhances a classic approach and makes it applicable to redundantly parametrized models and mobile systems. The method starts with formu-

lating the equations of motion in a form linear w.r.t. a set of dynamic parameters. This equations contain, as a consequence of the redundant coordinates, unknown constraining forces. The latter are eliminated from the motion equations by application of an orthogonal complement to the constraint matrix. As the identification performance depends on the used trajectories special attention is paid to the motion planning. This is highly important for determining a set of uniquely identifiable basis parameters and the computation of a reliable identification trajectory. Reliable refers thereby to a motion which, on the one hand, optimally excites the parameters but, on the other hand, prevents the vehicle from losing traction (wheel slippage). The overall approach is validated by experiments and shown to yield promising results.

An energy study of friction-induced vibrations in automotive brake systems

I. Iroz (University of Stuttgart), M. Hanss (University of Stuttgart), P. Eberhard (University of Stuttgart) 15:40

Despite all efforts made to improve the understanding of friction-induced vibrations, this mostly undesired phenomenon still represents a hard-to-resolve topic in many industrial applications. Amongst others, the squealing of automotive brake systems is displeasing for passengers, leads to high warranty costs, and with the introduction of electric mobility, increasingly affects the interior acoustics of vehicles. For decades, stability studies of friction-induced vibrations have relied on the well-known method of complex eigenvalue analysis. After linearizing the system around a sliding state, the delivered complex eigenvalues with a negative damping ratio reveal local instabilities. Besides not delivering vibration amplitudes, the global stability behavior may differ from the local one, and thus, the method tends to overestimate the number of instabilities.
Recently, elastic multibody systems based on the floating frame of reference approach have been applied to brake systems in order to overcome the issue of local instability and predict the vibration amplitudes in time domain. Moreover, the approach efficiently combines large rigid-body motions with small deformations, and consequently, time-consuming nonlinear analyses based on large finite-element models are avoided. For an accurate normal and tangential contact modeling, a master-slave approach with penalty parameters and Coulomb friction is used. As a result, the methods allows the investigation of the out-of-plane vibration for the nodes of interest, and, at a certain point in time, the occurrence of limit cycles is observed. In this way, after computing the spectrograms of the signals, the unstable frequencies of the squealing brake system are detected.
In this contribution, potential and dissipation energies at the contact interfaces are investigated. By considering the pressure applied to brake pads as the only energy source, and the dissipation by means of structural and contact damping, the complete energy of the system must remain constant. In a post-processing step, normal gaps, gap velocities and tangential forces are first retrieved from the contact algorithm. Thereafter, in normal direction, potential and dissipation energies for stiffness and damping penalties are calculated. Accordingly, in tangential direction, only a dissipation energy due to friction is computed. As a result, the energy study offers a deeper insight into the

dynamics of the brake system and further statements on the squeal propensity can be made.

S 1 : Multi-body dynamics

Wednesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 105

Real-time Trajectory Tracking of a Cable-driven Parallel Robot Using Servo-constraints

S. Otto (Technische Universität Hamburg), R. Seifried (Technische Universität Hamburg) 16:30

Cable robots are widely applicable for various tasks in the logistics industry and for large-scale manufacturing processes. Their ability to handle heavy payloads over a large working space is advantageous in the aforementioned applications. For such tasks, accurate trajectory tracking and positioning of the end-effector is an essential control objective for safety and performance reasons. This is especially challenging for underactuated cable robots since they possess less actuators than degrees of freedom. Trajectory tracking can be achieved by means of an inverse model based on servo-constraints. In this framework, the equations of motion are augmented by algebraic servo-constraints to enforce a specified trajectory of the system output. The resulting set of high index differential-algebraic equations (DAE) can be solved numerically to yield the feedforward control input. In this talk, it is shown that it is possible to solve the DAE problem in real-time, which makes the application to experimental setups straightforward. Stabilization of the tracking error can be achieved by a feedback controller which augments the feedfoward loop in a two degree of freedom control structure. In case of an accurate inverse model, the tracking errors are expected to be small. Thus, feedback control based on the linearized system dynamics is usually sufficient for stabilization.
The described servo-constraints method is applied to a cable robot consisting of an actuated trolley and a suspended payload. The load is attached to the trolley by four parallel cables, while each cable can be actuated individually. The cable robot is underactuated, since the load swinging represents an unactuated degree of freedom. Due to the kinematic loop imposed by the cables, the system is modeled in a DAE form. With the servo-constraints framework it is possible to enforce a specified trajectory for the center of gravity of the load. Taking into account that each rope can be actuated individually, there are additional degrees of freedom besides the load position that can be specified. For example, this can be utilized by including constraints on the load orientation. Constraining the load orientation is for example essential in balancing problems as considered here. The effectiveness of the described method is shown in simulations and experiments on a $13 \times 9\,\mathrm{m}$ cable robot test bench.

Motion by variation of the contact force on an inclined plane

P. Schorr (Ilmenau University of Technology), I. Zeidis, K. Zimmermann (Ilmenau University of Technology) 16:50

This paper describes non-classical locomotion based on the variation of the contact force. The motion of a locomotion system on an inclined plane is considered. The contact force between the locomotion system and the inclined plane can be influenced by the motion of internal masses. Therefore a mechanical model with two internal masses is introduced. The friction between the locomotion system and the environment is described by COULOMB's law. The motion of this locomotion system is investigated and analyzed by using the averaging method of BOGOLJUBOV and MITROPOLSKI. Furthermore the influence of different parameters on the locomotion characteristics like the direction of movement, the stationary velocity and the maximum inclination angle is shown. A prototype based on this locomotion principle is built up for experimental investigations. Additionally, simulations are used to analyze the locomotion system. The experimental values are compared to the theoretically results and confirm the variation of the contact force as an option to enable a controlled locomotion.

Variational integrator for constrained mechanical systems with pulsed disturbances and optimal feedback control

D. Glaas (University of Erlangen-Nuremberg), S. Leyendecker (University of Erlangen-Nuremberg) 17:10

Today, a lot of mechanical systems have to operate with an improved performance compared to equal constructions decades ago. To stay competitive, engineers need to optimise all aspects of a mechanical system including its optimal control and the handling of perturbations with feedback control.

An approach to minimize the control costs and ensuring a stable deviation control is the Riccati controller and we want to use it to control constrained dynamical systems (differential algebraic equations of Index 3). The discrete dynamics is described by a constrained variational integrator [2], a variant of a structure-preserving integration scheme. This yields, in combination with a discrete version of the Lagrange-d'Alembert principle, a forced constrained discrete Euler-Lagrange equation in a position-momentum form [1]. It is applied to three different coordinate choices, minimal coordinates $q_k \in \mathbb{R}^f$, $p_k \in \mathbb{R}^f$ with f being the number of degrees of freedom in the system, redundant coordinates $q_k \in \mathbb{R}^n$, $p_k \in \mathbb{R}^n$ and nullspace coordinates $q_k \in \mathbb{R}^n$, $p_k \in \mathbb{R}^f$.

The desired optimal trajectory (q_{opt}, p_{opt}) and according control input u_{opt} is determined solving the discrete mechanics and optimal control (DMOC) algorithm [3] based on the variational integrator. Then, during time stepping of the system with pulsed disturbances, the discrete Riccati feedback controller [4] yields the optimal deviation control input u_R, which is added to u_{opt}. As both DMOC and Riccati equations base on the same variational integrator, the resulting trajectory is symplectic.

Simulation examples apply several kinds of pulsed disturbances on mechanical system. Numerical results show that a stable handling of highly-nonlinear systems is assured. By comparing the feedback control effort, it reveals that all three coordinate parametri-

sations only differ slightly. Thus, a different choice of coordinates can be used in the feedback control and in the optimal control problem which might be useful in practice.

[1] E. Johnson, J. A. Schultz, and T. D. Murphey. Structured linearization of discrete mechanical systems for analysis and optimal control. IEEE Transactions on Automation Science and Engineering (2015), vol. 12, issue 1, 140–152.

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[3] S. Ober-Blöbaum, O. Junge, and J. E. Marsden. Discrete mechanics and optimal control: an analysis. ESAIM: Control, Optimisation and Calculus of Variations (2011), vol. 17, issue 2, 322–352

[4] B. D. O. Anderson and J. B. Moore. Optimal Control: Linear Quadratic Methods (1990). Prentice-Hall, Inc.

Optimal Control of Human Muscle-Actuated Motion

J. Fehr (Institute of Engineering and Computational Mechanics (ITM), University of Stuttgart), J. Fuhrer (Institute of Engineering and Computational Mechanics (ITM), University of Stuttgart), L. Gong (School of Life Sciences and Technology, Tongji University) 17:30

The question of how the brain planes locomotion is a highly treated one. To a great extent, motion is unconsciously realised by the central nervous system (CNS) making it difficult to deduce the underlying mechanisms which among others excite the human actuators – the muscles. A worthwhile resource to achieve further insight into this field are human computational models, since these models can provide a simulative access to values during an event which cannot be measured experimentally. Moreover, these models are beneficial for the design of prostheses, biomedical implants, the development of advanced rehabilitation devices or functional electric stimulations controllers and can be utilised to analyse energetics of human movement, athletic performance or joint replacement surgeries.

In this work, rigid multibody systems representing the human musculoskeletal system actuated by advanced Hill-type muscle models to simulate human movement within the program Neweul-M^2 are deployed [1]. Further, a forward dynamic approach is considered allowing to simulate human motion independently from pre-measured trajectories and besides enables to resemble the control of CNS, that is, the stimulation of muscles. It is suggested that movement paths arise implicitly through optimisation [2]. Hence, optimal stimulation patterns passing to activation dynamics are determined with regard to physiologically motivated objective functions by setting up and solving a constrained optimal control problem. More precisely, quadratic costs punishing the deviation to the final state position $\mathbf{x_f}$ and minimising the control effort, that is

$$J = (\mathbf{x} - \mathbf{x_f})^\top \mathbf{Q} (\mathbf{x} - \mathbf{x_f}) + \mathbf{u}^\top \mathbf{R} \mathbf{u}$$

with the control matrices **Q** and **R** are utilised. One advantage concerning the implementation within Neweul-M^2 is the possibility to apply well-elaborated and tested optimisation algorithms available with Matlab to solve optimal control problems. To gain more understanding, also nonlinear model predictive control is employed to obtain optimal stimulation patterns.
Within this study, the described framework is applied to treat different biomechanical movements, including reaching tasks of the arm or motion of the total human musculoskeletal system itself, where additionally the influence of external perturbations are considered. For validation, the arm model is compared with experimental data from [3, 2].

[1] J. Fehr, J. Fuhrer, C. Kleinbach, M. Hanss, P. Eberhard. Fuzzy-Based Analysis of a Hill-Type Muscle Model. PAMM (2016), 1, 16, 31–34.

[2] D.A. Kistemaker, J.D. Wong, P.L. Gribble. The cost of Moving Optimally: Kinematic Path Selection. Journal of Neurophysiology (2014), 8, 112 1815–1824.

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A Dynamic Programming Approach for Time-Optimal Path Following of Robots Considering Speed Dependent Torque Constraints

M. Oberherber (Johannes Kepler University Linz), H. Gattringer (Johannes Kepler University Linz), A. Müller (Johannes Kepler University Linz) 17:50

Time-optimal path following, i.e. of moving optimally along a specified geometric path, is a very important and well discussed problem in robotics. Nevertheless, most of the existing approaches concerning this topic neglect the speed dependent nature of torque constraints. This paper presents a method for taking such constraints into account within a dynamic programming approach. To this end, the problem is treated in parameter space. This allows for an optimal use of existing resources. Due to the demanding constraints precise mathematical models of the robots are indispensable. A satisfying match between model and real system can usually be achieved by parameter identification. For this purpose, it is a common way to derive the equations of motion using nominal parameters (masses, position of center of gravity, inertia and friction parameters), rewrite the equations in terms of linearly independent base parameters, and determine them with the help of measurements. Nevertheless, a parameterization of the motor torques has to be introduced in order to be able to consider their constraints within the optimization. In contrast to this, we will present a general toolchain, based on the Projection Equation that directly derives the base parameter representation and furthermore the parameters of the parametrized equations of motion. Simulation results and results for the experimental implementation on a real system are presented in this paper. The verifications

demonstrate the potential that can be exploited when considering constant, instead of speed dependent torque constraints for time-optimal robot trajectories.

S 1 : Multi-body dynamics

Thursday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 105

Screw Theory – A forgotten Tool in Multibody Dynamics

A. Mueller (Johannes Kepler University Linz) 14:00

In the fourth volume of the ZAMM, published in 1924, Richard von Mises introduced the 'Motorrechnung' (Motor Calculus) building on the earlier work of Robert Stawell Ball from the late 19th century on screw theory, Eduard Sudy's work on 'Dynamen', and Julius Plücker's work on line geometry. Since then screw theory has become a corner stone of modern kinematics. Kurt Magnus dedicated his Habilitation thesis to the application of motor calculus to the equations of motion (EOM) of rigid body systems. He made extensive use of the frame invariance of screws in order to derive the EOM represented in an arbitrary reference frame.
Recognizing that screws form the algebra of the Lie group of rigid body motions gave rise to compact and computationally efficient models in the last two decades governing the kinematics and dynamics of (rigid and flexible) multibody systems (MBS). This also provides a link to geometric mechanics and allows for application of geometric numerical integration methods on Lie groups. The coordinate invariance of Lie group formulations allows to derive various formulations that can be employed for different purposes. Yet screw theory has been largely ignored in MBS dynamics. In this paper the significance and potential of Lie group and screw theory for computational MBS dynamics is discussed. Recently proposed formulations are related to the classical MBS formulations and the advantages are explored. Special emphasize is given to the algorithmic and computational aspects.

Energy transfer from high frequency to low frequency modes in implicit time integration of nonlinear stiff mechanical systems

M. Arnold (Martin Luther University Halle-Wittenberg) 14:20

Implicit integrators with numerical damping combine artificial damping of undesirable high frequency solution components with accurate numerical solutions for the low frequency modes. For linear systems, both effects are decoupled and may be studied conveniently by a stability analysis for scalar test problems.
Similar results have been obtained for a class of strongly A-stable implicit Runge-Kutta methods being applied to mechanical systems with stiff potential forces $-\nabla\mathcal{U}_\varepsilon(q)$ that result from a potential $\mathcal{U}_\varepsilon(q) := \|g(q)\|_2^2 \,/\, \varepsilon^2$ with positive perturbation parameter $\varepsilon \ll 1$, see Ch. Lubich: *Integration of stiff mechanical systems by Runge-Kutta methods.* -

Zeitschrift für angewandte Mathematik und Physik ZAMP 44(1993)1022–1053.
In the present paper, we show that there is no equivalent result for Newmark type time integration methods. Even with numerical damping these methods suffer from a systematic energy transfer from high frequency modes to low frequency modes unless the initial values $q(t_0)$ are very close to the constraint manifold $\{\, q \,:\, g(q) = 0 \,\}$ of the corresponding reduced system that is obtained in the limit case $\varepsilon \to 0$. The results of the theoretical investigations are illustrated by numerical tests for a stiff pendulum.

Moreau-type integrators based on the time finite element discretization of the virtual action

G. Capobianco (University of Stuttgart), S. Eugster (University of Stuttgart), R. Leine (University of Stuttgart) 14:40

In this paper we derive and compare three integrators for nonsmooth mechanical systems by discretizing the principle of virtual action with finite elements in time. The weak variational form of the virtual action of a finite dimensional mechanical system

$$\delta A = \int_0^T \{\delta \dot{\boldsymbol{q}}^{\mathrm{T}} \boldsymbol{M} \dot{\boldsymbol{q}} + \delta \boldsymbol{q}^{\mathrm{T}} (\boldsymbol{f} + \boldsymbol{W} \boldsymbol{\lambda})\} \mathrm{d}t + \int_0^T \delta \boldsymbol{q}^{\mathrm{T}} \boldsymbol{W} \mathrm{d}\boldsymbol{\Lambda} + \delta \boldsymbol{q}(0)^{\mathrm{T}} \boldsymbol{p}_0 - \delta \boldsymbol{q}(T)^{\mathrm{T}} \boldsymbol{p}_T$$

includes the virtual action of the impulsive and nonimpulsive contact forces $\mathrm{d}\boldsymbol{\Lambda}$ and $\boldsymbol{\lambda}$, respectively. The non impulsive forces $\boldsymbol{\lambda}$ model the contact interactions during the impact free motion. The impulsive forces $\mathrm{d}\boldsymbol{\Lambda}$, given by a sum of Dirac point measures [1], model the contact interactions during impacts. Integrating the inertia term $\delta \dot{\boldsymbol{q}}^{\mathrm{T}} \boldsymbol{M} \dot{\boldsymbol{q}}$ by parts leads to the strong variational form of the virtual action δA of the mechanical system. The principle of virtual action states that δA vanishes for all virtual displacement fields $\delta \boldsymbol{q}$. A temporal finite element discretization of this variational principle, by choosing compatible virtual displacement fields, allows to deduce time-stepping schemes for nonsmooth mechanical systems [3]. The three integrators are derived by the discretization of either the weak or the strong variational form of the principle of virtual action with linear Lagrangian elements using different quadrature rules for the integral over the time t. The discrete constitutive laws for the contact forces are introduced as normal cone inclusions between the percussion, which combines the effects of both $\mathrm{d}\boldsymbol{\Lambda}$ and $\boldsymbol{\lambda}$ during a temporal element, and a kinematic quantity, which is given by pre- and post-impact velocities. This leads to Moreau–Jean's time-stepping scheme [2] and two other related schemes, which share many advantageous properties with the scheme of Moreau–Jean, as all schemes allow for multiple, simultaneous contacts and can overcome accumulation points. Moreover, the derived schemes show better longterm simulation behavior than Moreau–Jean's scheme.

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[2] Moreau, J. J. (1988) Unilateral contact and dry friction in finite freedom dynamics. *Nonsmooth mechanics and Applications*. Springer, Vienna.

[3] Capobianco G. and Eugster S. R. (2016) A Moreau-type Variational Integrator. *Proceedings in Applied Mathematics and Mechanics*. Wiley.

Variational integrators of mixed order for constrained and unconstrained systems acting on multiple time scales

T. Wenger (University of Erlangen-Nuremberg), S. Ober-Blöbaum (University of Oxford), S. Leyendecker (University of Erlangen-Nuremberg) 15:00

Mechanical systems with dynamics acting on different time scales, caused e.g. by different types or stiffnesses in potentials, are quite demanding with regard to adequate numerical methods. A stable integration of the fast motion requires a fine approximation. However, using the smallest necessary time-step comes along with unacceptable computational costs. As for the simulation of the slow motion, a coarse approximation is accurate enough, one established possibility is to separate the unknown configurations q into fast q^f and slow q^s degrees of freedom and to treat the components differently. For example multirate integrators use different time grids, in particular rather large time steps for the slow part and a fine grid for the fast part. However, the presented variational integrators of mixed order for unconstrained and for holonomically constrained systems work with only one time grid. Their construction bases on the Galerkin variational integrators in [1], where a polynomial is used to approximate the configuration together with an appropriate quadrature rule to approximate the action integral of the Lagrangian. The idea now is to approximate the components that act on different time scales via polynomials of different degrees, in particular a high degree polynomial for the fast part q^f and a low degree polynomial for the slow part q^s, and use quadrature rules of different orders to approximate the parts of the action, see [3] for unconstrained systems. The holonomic constraints $g(q) = 0$ are included by the Lagrange-multiplier theorem, where the term $g(q) \cdot \lambda$ augments the Lagrangian, with λ being the Lagrange-multiplier. To approximate the integral of the augmenting term, a polynomial is used for λ and a quadrature rule for the integral of $g(q) \cdot \lambda$, see [2]. We split the constraints into functions depending on the slow, fast and slow and fast degrees of freedom only, i.e. $g = [g^s(q^s), g^{sf}(q^s, q^f), g^f(q^f)]^T$. To avoid loosing accuracy in the approximation of the fast configuration, the integral of $(g^{sf}(q^s, q^f) \cdot \lambda^{sf})$ or $(g^f(q^f) \cdot \lambda^f)$, depending on the fast configuration, is approximated with high accuracy, meaning a polynomial of high degree to approximate the Lagrange-multiplier together with a quadrature rule of high order. Whereas when approximating the integral of $(g^s(q^s) \cdot \lambda^s)$, depending only on the slow configuration, a lower accuracy is sufficient. We use polynomials of different degrees to approximate λ^f, λ^{sf} and λ^s and appropriate quadrature rules of different orders. We show the performance of the integrators by means of numerical examples.

[1] S. Ober-Blöbaum and N. Saake, Advances in Computational Mathematics 41(6), 955–986 (2015).

[2] T. Wenger, S. Ober-Blöbaum and S. Leyendecker, PAMM 16, 775–776 (2016).

[3] T. Wenger, S. Ober-Blöbaum and S. Leyendecker, *Proceedings of the VII European Congress on Computational Methods in Applied Sciences and Engineering, ECCOMAS Congress*, Vol. 1, 1818–1831 (2016).

Conservative Time Advancement in the co-simulation of MBS/BE systems

J. Luthe (University of Rostock), J. Zierath (University of Rostock), C. Woernle (University of Rostock) 15:20

Extensive recent research shows the need for robust and fast contact algorithms in elastic multibody simulation (MBS) environments. Typical methods are either representing the elastic bodies on a basis of modally reduced Finite Element (FE) models on the one hand or setting up complete MBS/FE co-simulations on the other hand. However, these approaches lead to rather inaccurate local deformation results due to the need for global mode shapes, or to high computation times, respectively.

To circumvent these issues, an alternative method by coupling a commercial multibody program and a user-written boundary element (BE) routine is proposed in [4]. This method benefits from a rigorous DOF reduction of BE-formulation compared to FE-models, because only the surface needs to be discretised. Furthermore, as BE rely on a mixed formulation where both displacements and surface tractions are interpolated, they can reproduce high stress concentration – e.g. occurring during contacts – in an accurate way. To determine the contact state of two approaching bodies, bounding volume hierarchies are applied as an efficient way of collision detection. In order to prevent high and unphysical penetration depths of the involved bodies in the dynamic MBS/BE co-simulation, a small fixed integration step size is chosen throughout the whole simulation which results in large computation times in turn.

Based on the results of [4], this contribution presents a methodology of incorporating the concept of Conservative Time Advancement [1, 2] into an MBS/BE co-simulation using the commercial MBS program MSC Adams® with a variable step size integration method. When a collision is likely to take place, the integrator step size is refined adaptively in order to ensure that any initial penetration is below a prescribed threshold without missing any contact events. For this purpose, an enhanced version of the efficient GJK algorithm [3] is exploited to calculate the minimal distance of two approaching convex bodies, and a lower bound for the time of impact (TOI) is extrapolated on the basis of the bodies' current states. The TOI then represents the maximal permitted step size for the numerical integrator in the multibody environment. This simple methodology enables large step sizes at intervals with no contacts occurring and thus shorter computation times.

[1] B. Mirtich. Impulse-based Dynamic Simulation of Rigid Body Systems (PhD thesis). University of California, Berkeley, 1996.

[2] Murilo G. Coutinho. Guide to Dynamic Simulations of Rigid Bodies and Particle Systems. Springer London, 2013.

[3] C.J. Ong and E.G. Gilbert, Fast Versions of the Gilbert-Johnson-Keerthi Distance Algorithm: Additional Results and Comparisons, in IEEE Transaction on Robotics and Automation, Vol. 17, No. 4, August 2001.

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S 2: Biomechanics

Organizers: Gerhard A. Holzapfel (Graz University of Technology)
Udo Nackenhorst (Leibniz Universität Hannover)

S 2 : Biomechanics

Tuesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 101
Chair: Tim Ricken (TU Dortmund)

On a Tri-Scale and Multiphase Model for the Description of Perfusion coupled to Growth Effects in the Human Liver

N. Waschinsky (TU Dortmund University), D. Werner (TU Dortmund University), L. Lambers (TU Dortmund University), T. Ricken (TU Dortmund University) 14:00

The human liver regulates metabolism in a complex time depending and non-linear coupled function-perfusion-mechanism. The viability of the organ could be affected by a failure in the liver structure. A common damage is the excessive accumulation of fat in the tissue, known as a fatty liver. The growing fat has a high impact on the perfusion of the blood through the liver. The anatomy of the organ is characterized by a complex vascular system which changes on the different size scales from a vascular branching tree to microvessels, called sinusoids in liver lobules. To capture the interplay between fat deposition arising in the microstructure and the perfusion on the organ scale it is important to couple the processes on each scale. For this we present a computational model for the human liver which is composed of three coupled submodels for the organ, macro- and micro-scale. With the whole organ model we present the effect of growing fat vacuoles in the liver cells, which are inhomogenously distributed on organ-scale, as well as the total hepatic hemodynamics. The fat metabolism is evaluated on the micro-scale and leads to growth of the volume fraction in the liver lobule on the macro submodel. The growth leads to changes in the perfusion of the blood on the organ submodel.
On the organ scale we use a fluid mechanical approach calculating the perfusion in the branching system of the vascular tree. The vascular system starts with a single branch and subdivides into smaller vessels ending up in the portal triad - the interface of the

organ-scale to the macro-scale. With a computation of the vascular perfusion we provide information for the blood velocity and pressure as boundary condition. The macro-scale uses a homogenized mixture model for the simulation of important functionalities in the liver lobules as presented in [2, 3] including microperfusion and growth aspects. The approach uses the theory of porous media [1] to consider the biological tissue as a multiphase and multi-component structure including the liver tissue, the fat vacuoles, the blood, and components like glucose, free fatty acid, lactate, oxygen and glycogen. On the micro-scale we focus on metabolic processes which take place in the liver cells. We use a set of ordinary differential equations to evaluate the calculation of the microscopic components. The micro scale is weakly coupled to the macro scale.

[1] DE BOER, Reint. Theory of porous media: highlights in historical development and current state. Springer Science & Business Media, 2012.

[2] RICKEN, T., et al. Modeling function perfusion behavior in liver lobules including tissue, blood, glucose, lactate and glycogen by use of a coupled two scale PDE ODE approach. Biomechanics and modeling in mechanobiology, 2015, 14. Jg., Nr. 3, S. 515-536.

[3] RICKEN, Tim; DAHMEN, Uta; DIRSCH, Olaf. A biphasic model for sinusoidal liver perfusion remodeling after outflow obstruction. Biomechanics and modeling in mechanobiology, 2010, 9. Jg., Nr. 4, S. 435-450.

On a Multiscale and Multiphase Model for the Description of Hepatoxicity in Biological Tissue using the Example of the Human Liver

L. Lambers (Institute of Mechanics, Structural Analysis, and Dynamics; TU Dortmund University), N. Waschinsky (Institute of Mechanics, Structural Analysis, and Dynamics; TU Dortmund University), D. Werner (Institute of Mechanics, Structural Analysis, and Dynamics; TU Dortmund University), T. Ricken (Institute of Mechanics, Structural Analysis, and Dynamics; TU Dortmund University) 14:20

The liver is the most important organ related to metabolism processes in human beings. A central task of the human liver is the detoxification of toxic metabolites since excessive amounts of several medications can cause damages in the liver structure which can lead up to acute liver failure.

One example for a medicine which can cause hepatoxicity is analgesic Paracetamol (Acetaminophen). The toxic metabolites of the Paracetamol are normally depleted by conjunction with the internal glutathione. If the concentration of hepatic glutathione is exhausted, the glutathione are no longer capable of binding the molecules and the reactive metabolites react with cellular proteins causing liver necrosis.

The now developed model is an extension of a previous published work, where a multicomponent, poro-elastic multi-phasic and multi-scale function-perfusion approach has been presented, cf. [2, 3, 4].

In addition, the depletion of toxic medicines causing cell damage through an acute overdose is supplemented using the example of the analgesic Paracetamol (Acetaminophen). Furthermore the kinetic relations of the Paracetamol and the internal metabolite glutathione are appended.
The human liver consists of liver lobules, which contain small cells, called hepatocytes, where the metabolism takes place. Therefore, the toxic metabolites, just like other nutrients and substances, are initiated in the liver with an anisotropic blood flow via the sinusoids (slender capillaries sited between the periportal field and the central vein). As the structure of liver lobules is extremely complex, we use a multi-component mixture theory based on the Theory of Porous Media (TPM), see [1]. Applying the TPM, the allocation of the sinusoids as well as the complex distribution of the hepatocytes can be homogenized.
The computational model consists of a tetra-phasic component body, composed of a porous solid structure φ^{S}, fat tissue with the ability of growth φ^{FL}, a liquid phase representing the blood φ^{L} and a solid phase φ^{N}, which characterizes the damaged necrotic cells. The phases present a carrier phase φ^{α}, also called solvent, and solutes $\varphi^{\alpha\beta}$, representing microscopic components, that are solved in the solvent and consist of the nutrients responsible for the metabolism in the liver. To calculate the processes and describe the production, utilization and storage of the metabolites, an embedded set of coupled ordinary differential equations (ODE) is used.

[1] DE BOER, R. [2002], "Theory of porous media: highlights in historical development and current state", Springer Science & Business Media.

[2] RICKEN, T. ET AL. [2015], "Modeling function perfusion behaviour in liver lobules including tissue, blood, glucose, lactate and glycogen by use of a coupled two scale PDE ODE approach", Biomechanics and modeling in mechanobiology, 14. Jg., Nr. 3, S. 515-536.

[3] RICKEN, T., DAHMEN, U., DIRSCH, O. [2010], "A biphasic model for sinusoidal liver perfusion remodeling after outflow obstruction.", Biomechanics and modeling in mechanobiology, 9. Jg., Nr. 4, S. 435-450.

[4] WASCHINSKY, N. [2016], "On a bi-scale and tri-phasic model for the description of growth in biological tissue using the example of human liver", PAMM Proc. Appl. Math. Mech. 16, S. 109-110.

Towards a virtual mechanical human brain

A. Wagner (University of Stuttgart), D. Fink, P. Schröder (Institute of Applied Mechanics (CE)), W. Ehlers (University of Stuttgart) 14:40

It is supposed that the vision of an integrated Overall Human Model (OHM) can be realised by the combination of isolated models. By this means, a so-called OHM-toolbox contains these models, which need to be extended and/or linked to each other depending on the desired use. However, this implies the need to bridge over several length and

time scales as well as to combine different physical effects and numerical approaches. In this regard, the proposed contribution is related to the description of one part of this toolbox, namely, the overall mechanical behaviour of human brain tissue. As an application-driven organ model, it can substantially contribute to a holistic understanding of various complex processes, such as the study of brain-tumour treatment.

However, several capabilities are requested to achieve a simulation environment which can serve as a virtual testbed for reliable predictions of clinical interventions. A basic prerequisite is a sound theoretical modelling framework. The contradiction between the enormous microscopical complexity of the multicomponent brain-tissue aggregate and the aim to consider problems on the scale of centimetres motivates the application of the well-known Theory of Porous Media (TPM). In particular, the model proceeds from an anisotropically deformable solid skeleton constituted by tissue cells and vascular walls. This solid skeleton is perfused by two mobile but separated pore liquids. These are the blood in the vascular system of the brain and the interstitial fluid in the interstitial fluid space. Moreover, these fluids can themselves be treated as real mixtures of multiple components if this is required, such as for the description of drug applications or tumour growth processes.

Moreover, important aspects for a reliable personalised description are discussed in this presentation. This implies the inclusion of an enormous amount of medical data, obtained from patient-specific imaging procedures. In particular, the geometrical representation of the brain's shape and constitution can be gained from non-invasive imaging, such as (micro) Computed Tomography (CT), Magnetic Resonance Imaging (MRI) or Magnetic Resonance Angiography (MRA). Moreover, material properties such as anisotropic permeability conditions of the brain tissue can be estimated from diffusion-weighted Magnetic Resonance Imaging (DTI). Besides the mechanical behaviour, it is often necessary to extend the model complexity via the inclusion of non-mechanical measures via systems-biological approaches. In addition, a key issue for an accompanying use during clinical routine is the required computation time. Due to the complex model, the numerical solution is typically extremely costly in terms of time. In order to transfer the model to a clinical application, there are promising pathways for a numerical acceleration, such as model-reduction techniques. Therefore, necessary adaptations to apply state-of-the-art model-reduction techniques, such as the POD-DEIM, to the nonlinear brain-tissue model are discussed.

Data-driven simulation of metastatic processes within brain tissue

P. Schröder (Institute of Applied Mechanics (CE)), A. Wagner (University of Stuttgart), W. Ehlers (University of Stuttgart) 15:00

Metastases crucially disturb an affected organ and compromise its functionality, for example, by increasing the stress and disrupting cells. In this contribution, the behaviour of lung metastases within the brain tissue is described in terms of a continuum-mechanical model. Therefore, multicellular cancer-cell-spheroid experiments are incorporated to

step towards a data-driven model.

In particular, lung cancer growth and atrophy are of special interest. In the initial step of the tissue invasion, cancer cells may pass the blood-brain barrier (extravasation) and invade the surrounding tissue. In the following, a sufficient nutrient supply triggers the formation of micrometastases originated from the cancer cells. Furthermore, the cancer cells stimulate blood-vessel sprouting leading to large interveined metastases. A promising option to treat metastases and its consequences is to infuse a therapeutic agent into the extravascular space of the brain tissue in the vicinity of the metastasis site.

The introduced processes are described in the framework of the Theory of Porous Media (TPM). This macroscopic multi-phasic modelling approach is based on a volumetric homogenisation of the microscopic structure over a representative elementary volume. Consequently, superimposed and interacting continua of the constituents are obtained which can be modeled in a continuum-mechanical approach. In particular, the constituents are an elastic solid skeleton (brain cells and metastases) and two immiscible pore liquids (interstitial fluid and blood). Moreover, the pore liquids are themselves real mixtures of miscible components. In particular, the components of the blood are the solvent and the cancer cells, which may extravasate into the interstitial fluid. In addition, the interstitial fluid contains nutrients and a therapeutic agent. The metastatic processes of atrophy, growth, extravasation and angiogenesis are described by mass exchange terms. To demonstrate the feasibility of the data-driven model, the specific growth rates are related to cancer cell experiments about growth, starvation and drug infusion. Thus, the experimental observations on the microscale are embedded in the macroscopic model.

The governing equations of this model are provided by the overall momentum balance and the adapted mass balances relations. Therefore, the primary variables are the solid deformation, the liquids' pore pressures and the concentrations of the solved components. Numerically, the partial differential equations are solved monolithically, applying the inhouse finite-element package PANDAS. The discretisation in space is carried out by extended Taylor-Hood elements. Furthermore, the model is discretised in time by an implicit Euler time-integration scheme.

Finally, numerical simulations of metastatic processes are performed, based on experimental data, to observe the behaviour of the multicellular cancer-cell-spheroids within brain tissue.

Heat transfer in multi-phase porous media with application to cancer detection

A. Niedermeyer (RWTH Aachen University), Y. Heider (RWTH Aachen University), M. Stoffel (RWTH Aachen University), B. Markert (RWTH Aachen University) 15:20

Over 8 million people die each year from cancer [1]. As early diagnosis may improve outcomes, the ultimate goal of this research project is to develop a method for cancer detection, which is accurate, inexpensive and not harmful to health.

For this purpose, a thermographic camera together with computational modelling can be used to measure an internal heat source caused by cancerous tissue. In particular, thermographic images of the surface temperature distribution and coupled thermomechanical modelling are combined. Porous media theories are well-suited for the detailed modelling of hydrated biological tissue and therefore used in this approach, see [2] among others.
In a first step, a simplified computational model is developed which incorporates heat transport in a heterogeneous medium representing biological tissue. The computational model calculates the bulk and surface temperature distribution. Secondly, the computational model is compared to thermographic images of a specimen. The thermographic images are acquired by means of a high-resolution infrared camera available at the Institute of General Mechanics [3].

[1] Stewart, B. W., Wild, C. P.: *World Cancer Report 2014*, International Agency for Research on Cancer (2014).
[2] Markert, B.: *Coupled thermo- and electrodynamics of multiphasic continua*, Advances in Extended and Multifield Theories for Continua Lecture Notes, Applied and Computational Mechanics 59, p.129-52 (2011).
[3] Lamjahdy, A. et al.: *The cyclic thermomechanical coupled problem of thermal gradients in friction railway disc brakes*, PAMM 14(1), p.461–2 (2014).

Effective compressibility and chemo-mechanics of soft tissue membranes

A. Ehret (Empa), A. Stracuzzi (ETH Zürich), K. Bircher (ETH Zürich), E. Mazza (ETH Zürich) 15:40

Based on the high water content of soft biological tissues, their compressibility is typically considered small and their mechanical behaviour is treated in the framework of near or full incompressibility. Recent experiments on soft tissue membranes, however, revealed large lateral contraction within and perpendicular to the membrane plane [1, 2], causing substantial reduction of volume both in simple and equibiaxial tension tests, enabled by efflux of water. Although both this strong effective compressibility of the tissues and the reduction of volume that accompanies tensile load states, in which the hydrostatic pressure is negative, seem counterintuitive, we show in this contribution that these phenomena are in agreement with thermodynamics and are related to a strong chemo-mechanical coupling between the constituents of these membranes. Employing theories for bi-phasic and swelling media, these characteristics are rationalized by constitutive models and compared with experimental data.

[1] A. Mauri et al, *Acta Biomater* 11:314-323, 2015

[2] M. Perrini et al, *J Biomech Eng* 137:061010, 2015

S 2 : Biomechanics

Tuesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 101
Chair: Oliver Röhrle (Universität Stuttgart)

Investigating human thumb models via their range of motion volumes

U. Phutane (FAU Erlangen-Nürnberg), M. Roller (Fraunhofer Institut für Techno- und Wirtschaftsmathematik), S. Björkenstam (Fraunhofer-Chalmers Centre), S. Leyendecker (FAU Erlangen-Nürnberg) 16:30

The grasping activity is possible due to the unique design of the human thumb and its complex motions viz. apposition, opposition etc. To simulate these motions, a physically correct model of the thumb is necessary. The thumb anatomy is made of three bones and three joints, namely the carpometacarpal (CMC) joint between the carpal bone and the first metacarpal bone, the metacarpophalangeal (MCP) joint between the first metacarpal and the proximal phalanx bone and the interphalangeal (IP) joint between the proximal and distal phalanges.

The CMC is a saddle joint with rotations of flexion-extension (FE) and adduction-abduction (AA) and has been implemented in biomechanical models as a universal joint [1]. However, cadaver studies [2] have shown that the CMC (and also the MCP) joint is composed with two axes of rotations which are non-orthogonal and non-intersecting, unlike a universal joint. Also, such a joint configuration is necessary to develop correct thumb tip forces [3]. Here, we develop a multibody model, similar to [4], of the thumb with two degrees of freedom (FE and AA) each for the CMC and the MCP joints and one degree of freedom (FE) for the IP joint. The bone dimensions are obtained from [6] and the location and the orientation of the joint axes are taken from [2].

To validate the realistic behavior of the model, we perform a two-fold validation test. Firstly, we plot the point cloud of the work-space created by the tip of the thumb by moving the thumb kinematically in all its degrees of freedom and then calculate the volume using alpha shapes. There are two sets of limits on the range of motion (ROM), namely the maximum ROM and the grasp ROM. The grasp ROM limits are smaller than the maximum ROM and it yields lesser volume than the maximum ROM. This volume reduction is a kinematic measure for a thumb model. We calculate the volume reduction for five different thumb models (described in [6]). The volume reduction for the thumb models from our simulations is in the range of 71% to 75%. We compare these values with data from literature [5], wherein the volume reductions vary between 68% and 76%.

Secondly, we compute the axial rotation of the thumb CMC joint in different postures, which is an outcome of the thumb in FE and AA. We compare the axial rotation of the first metacarpal for different FE and AA rotations with values from literature [1]. The axial rotation simulation results also lie within the standard deviation limits of the literature values. The results for the two validation tests are in close agreement with the literature values and consequently the thumb model can be said to have been validated

kinematically.

[1] Cooney, William P and Lucca, Michael J and Chao, EY and Linscheid, RL. The kinesiology of the thumb trapeziometacarpal joint. The Journal of Bone and Joint Surgery, 63(9):1371-1381, 1981.

[2] Hollister, Anne and Buford, William L and Myers, Loyd M and Giurintano, David J and Novick, Andrew. The axes of rotation of the thumb carpometacarpal joint. Journal of Orthopaedic Research, 10(3):454-460, 1992.

[3] Valero-Cuevas, Francisco J. and M. Elise Johanson, and Joseph D. Towles. Towards a realistic biomechanical model of the thumb: the choice of kinematic description may be more critical than the solution method or the variability/uncertainty of musculoskeletal parameters. Journal of biomechanics, 36(7):1019-1030, 2003.

[4] Maas, Ramona and Leyendecker, Sigrid. Biomechanical optimal control of human arm motion. Journal of Multi-body Dynamics, 227(4):375-389, 2013.

[5] Dermitzakis, Konstantinos and Andreas Ioannides, and Hwai-ting Lin. Robotic thumb grasp-based range of motion optimisation. 35th Annual International Conference of the IEEE Engineering in Medicine and Biology Society (EMBC), pp. 3163-3166, 2013.

[6] Santos, Veronica J and Valero-Cuevas, Francisco J. Reported anatomical variability naturally leads to multimodal distributions of Denavit-Hartenberg parameters for the human thumb. IEEE Transactions on Biomedical Engineering, 53(2):155-163, 2006.

Development of a movement generation algorithm for Finite Element Human Body Models

O. Martynenko (University of Stuttgart), S. Schmitt (University of Stuttgart), A. Bayer (University of Stuttgart), J. Blaschke (Daimler AG), C. Mayer (Daimler AG) 16:50

In the near future one aim of the automotive industry is an autonomous self-driving car with free sitting posture for the occupant. He or she will be allowed to do a lot of different movements in addition to nowadays steering. This situation directly affects the car safety systems development. Presently, their main focus is the in-crash scenario and in the future it will move more to pre-crash. There, re-active and pro-active response of the driver to the road situation before possible impact should be taken into account. One option to contribute to this action is to implement general movement generation algorithms for virtual Finite Element Human Body Models (FE HBMs). Such models are used currently for in-crash simulations with the intention to extend their application field to pre-crash simulations.

For this method, physiologically motivated and experimentally validated models are required to predict the dynamic interplay of the neural controller with the musculoskeletal biophysics. Various model representations with different levels of details already were implemented and could be found in literature. This numerical study implements HBMs activation via insertion of 1D Hill-type elements for each muscle represented with individual parameters for material, contraction and activation dynamics. The modelling approach is based on results of a forward dynamics full human multi-body (MB) model simulation [1], driven by 260 muscle-tendon units (MTUs) modelled as Hill-type muscles consisting of: a contractile element (CE), a serial-elastic element (SEE), a serial-damping element (SDE) and a parallel-elastic element (PEE) [2]. The activation dynamics was modelled with a closed-loop λ-control algorithm, which initiates the target position change from one position to another [3].
Preliminary results of the algorithm show that 1D Hill-type elements could act as a motor for FE HBM [4] and this improved model could be used for new active integrated safety systems development. Some further investigations need to be done in the direction of finding optimal number of Hill-type elements per muscle and muscle path deflection with correct tendons implementation.

[1] Rupp, T.K., Ehlers, W., Karajan, N., Guenther, M., Schmitt, S., A forward dynamics simulation of human lumbar spine flexion predicting the load sharing of intervertebral discs, ligaments, and muscles. *Biomech. and Modeling in Mechanobiology* 14(5), pp. 1081-1105, 2015. DOI: 10.1007/s10237-015-0656-2.

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[3] Rockenfeller, R., Guenther, M., Schmitt, S., Goetz, T., Comparative Sensitivity Analysis of Muscle Activation Dynamics. *Computational and Mathematical Methods in Medicine*, vol. 2015, pp.1-16, 2015. DOI: 10.1155/2015/585409

[4] Martynenko, O., Blaschke, J., Mayer, C., Schmitt S., (2016) Computer simulation of steering operations using activated THUMS and LS-Dyna. Proceedings of CARHS: Human Modeling and Simulation in Automotive Engineering conference, Heidelberg, Germany.

A key to high-amplitude movement synthesis: the muscle lever arm

M. Hammer (Universität Stuttgart), S. Schmitt (Universität Stuttgart), M. Günther (Universität Stuttgart), D. Haeufle (Universität Tübingen) 17:10

Pulling actuators play an important role in biomechanical simulations. In most animals, muscles are the actuators exerting torques onto the joints. These torques highly depend on the muscles' line of action or, in other words, muscle lever arms. Common methods focus either on single-joint movements, on two-dimensional problems, or on imitating physiological lever arms only in a small working range. However, especially in complex

multibody simulations, where a reduced descriptions of muscles as elastic bands is used, a correct representation of lever arms is mandatory for a large range of joint angles for all degrees of freedom. To address these issues, we developed a new design and computational algorithm for modeling the path of linear pulling actuators. The method is based on finding the minimum potential energy path while the actuator is lead through a small number of two-dimensional shapes. It allows for multiple degree of freedom and high-amplitude movements as well as combinations of both, ensuring reasonable lever arms at all possible joint configurations even for muscles spanning more than one joint. We applied this method to a multibody model of the human musculoskeletal system.

An approach to generate data of noncontact ACL injury prone situations by computer simulation

R. Eberle (University of Innsbruck), D. Heinrich, P. Kaps, W. Nachbauer, M. Oberguggenberger 17:30

An anterior cruciate ligament (ACL) injury is a common injury in sports and implies in particular high surgery costs, long and intensive rehabilitation and bad influence on patient's quality of life. Most ACL-injuries occur without physical contact between athletes (noncontact injuries). To prevent noncontact ACL-injuries it is necessary to understand the underlying injury mechanism. Kinematic data of noncontact injury prone situations provide important information for studying the underlying injury mechanisms. However, these data are rare. In this contribution, an approach is presented to generate kinematic and kinetic data of noncontact ACL-injury prone situations on a computer by a musculoskeletal simulation model using kinematic data of a non-injury situation (reference situation) and the method of Monte Carlo simulation.

Based on the reference situation a series of n perturbations is generated (Monte Carlo simulation). In detail, the initial kinematic data of the reference situation $q_{\text{reference}}(0)$ are randomly perturbed by adding random numbers ϵ to kinematic coordinates

$$q(0) = q_{\text{reference}}(0) + \epsilon.$$

With these perturbed data, the following optimal control problem (OCP) is solved:

Minimize objective function

$$\min_u J(u)$$

w.r.t. control variables u subjected to the musculoskeletal simulation model:

$$f(x, \dot{x}, u) = 0$$

and fixed initial conditions.

The perturbed simulations with ACL tensile forces higher than a specified threshold are collected and classified as injury prone situations.

The approach was successfully applied to generate injury prone landings after a jump in downhill ski racing. The obtained injury prone landings were consistent with video recordings in other studies.

A homogenisation method for the multiscale modelling of transversely isotropic skeletal muscle tissue

C. Bleiler (University of Stuttgart), P. Ponte Castañeda (University of Pennsylvania), O. Röhrle (University of Stuttgart) 17:50

Skeletal muscle tissue shows a wide variation in its mechanical response for different persons or different muscle types of one single person. These distinct mechanical properties are due to variations in the microstructure of the material. For skeletal muscles, especially the arrangement and the stiffness of collagen fibres in the connective tissue define the macroscopic passive stiffness, while the sarcomeres (contractile units) enable an active contractility of the muscles. Phenomenological models lack the ability to take into account such microstructural variations in a natural way and need to be fitted to experimental data, which is, however, not available for every desired muscle type.
Thus, this work presents a homogenisation-based multiscale model for skeletal muscle tissue which enables to include microstructural properties in a continuum-mechanical framework. The underlying homogenisation is done by means of the tangent-second-order (TSO) method, which is appropriately extended in order to account for the transversely isotropic behaviour of the muscle material. Moreover, an angular-integration model is embedded for a comprehensive description of the connective tissue. Concluding, the presented model allows to directly include microstructural-based material properties on the continuum-mechanical macroscale and yet avoids the expensiveness of computational homogenisation methods, like FE^2, by using well-founded analytical homogenisation techniques.

Wobbling masses in human legs: they cost but pay off

S. Schmitt (University of Stuttgart), M. Guenther (University of Stuttgart), D. Haeufle (University of Tuebingen) 18:10

Humans seem biomechanically unique in the animal kingdom. Rather than the use of just two straight legs, or even just one as in sleeping birds, it is the amount of muscle mass located in the legs that makes up this human uniqueness. As muscle masses are soft tissue attached to the skeleton they start to "wobble" when the bones are mechanically excited by impacts. That is, they are exposed to visco-elastic forces which induce oscillatory soft tissue movements relative to the bones and come along with energy dissipation. As the latter is expected to scale with the mass portion we asked for absolute numbers: how much energy is dissipated by human wobbling masses after a leg impact? We calculated these numbers in human running by estimating the wobbling mass kinematics from high-speed imaging sequences. The comparison to axial leg work and joint energy balances during ground contact provides a measure of relevance for the irreversible energy loss by leg wobbling masses. We discuss functional explanations for the acquiescence of such a uniquely high amount of wobbling masses in the leg. We also try and explain how

they yet pay off although any significant amount of irreversible energy loss like wobbling mass dissipation would seem inefficient and thus expectably avoided as good as possible by nature.

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[4] S. Schmitt and M. Günther, Archive of Applied Mechanics 81(7), 887–897 (2011).

S 2 : Biomechanics

Wednesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 101
Chair: Bernd Markert (RWTH Aachen)

Experimental and computational analysis of human articular cartilage under mechanical loading: functional MR imaging vs. constitutive modelling of biomechanical tissue properties

K. Linka (RWTH Aachen University, Department of Continuum Mechanics), M. Itskov (RWTH Aachen University, Department of Continuum Mechanics) 14:00

Osteoarthritis (OA) is a widespread clinical condition. In spite of utmost clinical relevance in terms of diagnosis and subsequent treatment, the detection of early disease stages remains diagnostically challenging. All these stages, the macroscopic appearance of the cartilage remains unchanged, while the elastic stiffness of the tissue decreases. Therefore, one promising non-invasive approach is to functionally assess the tissue's response to loading by serial multiparametric magnetic resonance (MR) imaging mapping of distinct tissue properties such as T1ρ (a marker of proteoglycans) or T2 (a marker of tissue water and collagen content) [1]. However, it is not clear which cartilage component, i.e. tissue water or the extracellular matrix consisting of primarily type-II collagen and proteoglycans, contributes to the tissue functionality. Further elucidation of the individual components' contributions to the cartilage response to mechanical loading would provide a scientific basis for the future clinical translation of functional MRI techniques in the detection of early OA

Functional maps (of MRI parameters such as T1ρ and T2) were generated of histologically intact cartilage samples using a clinical 3.0-T MR imaging system as before [1].

Using displacement-controlled static indentation loading, serial MRI mapping was performed at different strain levels.

To this end, an anisotropic hyperelastic constitutive model of fiber-reinforced materials [2] was utilized to model cartilage properties and their associated response to loading. In this regard, the volumetric part of the strain energy function was studied in detail and varied fiber alignments (both intra- and inter-sample-wise) were modeled. Computational analysis revealed collagen fiber reorientation and volumetric changes due to indentation loading, which are further compared to the MR results. Possible relations between the parameter map changes and the components of the ECM are discussed.

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[2] A.E. Ehret and M. Itskov, A polyconvex hyperelastic model for fiber-reinforced materials in application to soft tissues. Journal of Materials Science. (2007) 42:8853-8863.

Mechanobiological processes of tissue engineered cartilage replacement materials

J. Nachtsheim (Institute of General Mechanics), G. Dursun (Institute of General Mechanics), M. Stoffel (Institute of General Mechanics), B. Markert (Institute of General Mechanics) 14:20

Articular cartilage is a highly complex and sensitive part of the musculoskeletal system. Its degradation due to wear is challenging regenerative medicine. Owing to its poor self-healing abilites, small local defects often require surgical treatment. First clinical studies have revealed cell-free collagen implants to be a promising replacement material [1]. In vivo, the scaffolds are colonised by cells and remodelling processes optimise the characteristics of the substitute. In this study, a bioreactor system is used allowing to emulate these processes in vitro. In a first step, cell-migration is studied and the influence of an external mechanical stimulation is analysed. Additionally, a material model is applied to simulate the time-dependent behaviour of the replacement material [2].

[1] Schüttler, K.F., Pöttgen, S., Getgood, A., Rominger, M.B., Fuchs-Winkelmann, S., Roessler, P.P., Ziring, E., and Efe, T.: *Improvement in outcomes after implantation of a novel polyurethane meniscal scaffold for the treatment of medial meniscus deficiency*, Knee Surgery, Sports Traumatology, Arthroscopy, 23(7), pp.1929-1935. (2015).

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Homogenized constrained mixture models: a new approach to growth and remodeling of soft biological tissues

C. Cyron (TU München), F. Braeu (TU München), R. Aydin (TU München) 14:40

Growth and remodeling of soft biological tissues play important roles in many areas of biomechanics and biomedical engineering. Simple kinematic growth models are still widely used. However, they cannot represent the simultaneous growth and remodeling processes of several constituents (such as collagen, elastin, and smooth muscle) in the tissue. To overcome this deficiency, so-called constrained mixture models were developed in the early 2000s, inspired by multi-network theory. The mechanical and mathematical basis of these models is physiologically much more realistic than the one of simple kinematic growth models and they can capture features of soft tissue growth and remodeling that are beyond the scope of simple kinematic growth models. However, their complexity and computational cost are very high. Here we present a new class of models for growth and remodeling of soft biological tissues, the so-called homogenized constrained mixture models. These retain the realistic micro-mechanical basis of classical constrained mixture models based on multi-network theory. However, their complexity and computational cost are comparable to the ones of simple kinematic growth models. This way, homogenized constrained mixture models combine in a favorable way the advantages of the two currently dominant approaches to soft tissue growth and remodeling, that is, of kinematic growth models on the one hand and of constrained mixture models based on multi-network theory on the other hand. Homogenized constrained mixture models thus bear great promise to serve as a fast and powerful workhorse in future computational studies of growth and remodeling in soft biological tissues.

Modelling the contraction properties of smooth muscle cells in bladder tissue

R. Seydewitz (TU Braunschweig / Institut für Festkörpermechanik), M. Böl (TU Braunschweig / Institut für Festkörpermechanik) 15:00

The urine bladder is a hollow organ for the storage and release of urine. During filling the bladder volume can reach values up to several hundred percent which causes high deformations in the tissue while maintaining a nearly constant pressure. This remarkable behaviour is due to the complex microstructure in conjunction with a multi-layered composition of the tissue. For the release of urine smooth muscle cells in the muscle layer contract leading to contraction of the whole bladder. Generally smooth muscle cell contraction can be initiated by different excitation-contraction pathways. The 'electrochemical' coupling is based on the depolarisation of the membrane potential by electrical stimulation where extracellular calcium ions enter the cell via voltage-gated channels in the cell membrane. The increase of the internal calcium concentration acts as a trigger for smooth muscle contraction. Alternatively, stretch sensitive and non-specific ion channels trigger 'mechano-electrochemical' coupling by increasing the permeability for cations to depolarise the membrane potential and to allow the influx of extracellular calcium ions. In order to obtain a better understanding of the contraction properties during storage and release of urine a three-dimensional multi-field phenomenological model

was developed and implemented in the finite element method. Within the modelling approach, the membrane potential is governed by a FitzHugh-Nagumo type equation, triggering also the different excitation-contraction pathways. Accounting the influence on the deformation, mechanically important layers are modelled as separate material layers. Finally, the model is applied to different examples with complex boundary conditions to demonstrate the capability of the proposed model to mimic the physiology of bladder contraction.

On the mechanical characterisation of oocytes

M. Böl (TU Braunschweig, Institute of Solid Mechanics), J. Dittmann 15:20

To date, no experimental methods are available to completely characterise individual oocytes mechanically. Accordingly, structural, mechanical and physiological knowledge about the three-dimensional cell mechanical behaviour is lacking so that an adequate three-dimensional model could so far not be established. In order to bridge this knowledge gap this work focuses on micromechanical experiments to characterise the mechanical behavior of oocytes. In doing so, experiments on oocytes are performed under visual observation and consequently allowing the identification of material parameters in a more expressive way. From the mechanical point of view, the zona pellucida is of particular importance since it is the main load bearing component of oocytes and has a very interesting microstructure and in addition, their mechanical properties change significantly during fertilisation. The zona pellucida exhibits a strong anisotropic microstructure resulting from the specific protein distribution. These morphological features are visually identified in this work and can be included in the model development. Summarising, within this work different mechanical and optical experiments are realised to identify the mechanical behaviour of the different components (zona pellucida, ooplasma) of oocytes. These characteristics are the basis for a proper model development. Further, appropriate material parameters have been identified by the use of the inverse finite element method.

S 2 : Biomechanics

Wednesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 101
Chair: Daniel Balzani (TU Dresden)

Steps towards more realistic FSI-simulations for coronary arteries

S. Fausten (Institute of Mechanics, University of Duisburg-Essen), D. Balzani (Institute of Mechanics and Shell Structures, TU Dresden), A. Heinlein (Mathematical Institute, University of Cologne), A. Klawonn (Mathematical Institute, University of Cologne), O. Rheinbach (Institute of Numerical Mathematics and Optimization, TU Freiberg), J. Schröder (Institute of Mechanics, University of Duisburg-Essen) 16:30

Fluid-Structure Interaction (FSI) is a research field with a broad variety of applications.

Here, we focus on its applications in the field of hemomechanics, in detail the simulation of coronary arteries, where the interaction of the blood flow and the vessel wall is of major interest. In our ongoing research a simplified benchmark problem, which is described in [1], has been used for the simulation of coronary arteries. The benchmark problem depicts the influence of different element formulations onto the stress approximation quality as well as the necessary mesh size needed to obtain converging FSI solutions. Nevertheless, due to the simplified geometry and composition of the structure it lacks applicability to real life problems and thus more realistic simulation setups should be considered. Therefore, two steps towards more realistic FSI-simulations for coronary arteries are proposed here. On the one hand the tissue surrounding the artery is taken into account, i.e. the perivascular adipose tissue. It is included into the simulation in order to obtain more realistic structural boundary conditions. This extends the benchmark problem and thus the results are compared with the results from [1]. Here, massive parallel computing and a novel two-level overlapping Schwarz method are applied in order to deal with the increasing complexity of the boundary value problem, cf. [2]. On the other hand a short segment of a realistic geometry is considered. For this purpose, the so-called virtual histology is taken into account, which provides information regarding a stack of axially distributed two-dimensional cross-section images from which the individual components of the arterial wall such as the media, adventitia and plaque can be segmented, cf. [3]. Even though, the segment is not long enough to establish realistic flow conditions for the fluid, additional complexity is introduced by the geometry and the different material components and therefore serves as a good starting point for further FSI simulations with realistic coronary geometries. Here, the focus is on the in- and outflow conditions for the fluid, which pose a special challenge due to the irregular in- and outflow areas. For both approaches the structure is modeled by the well established material model introduced in [4]. The numerical simulations are performed, using the Open-Source project LifeV, in particular a code which has been developed in cooperation with the group of Prof. Quarteroni from the EPF Lausanne.

[1] D. Balzani, S. Deparis, S.Fausten, D. Forti, A. Heinlein, A. Quarteroni, O. Rheinbach, J. Schröder, Numerical modeling of fluid–structure interaction in arteries with anisotropic polyconvex hyperelastic and anisotropic viscoelastic material models at finite strains. *International journal for numerical methods in biomedical engineering*, DOI:10.1002/cnm.2756, 2015.

[2] A. Heinlein, A. Klawonn, O. Rheinbach, A parallel implementation of a two-level overlapping schwarz method with energy-minimizing coarse space based on trilinos. *SIAM Journal on Scientific Computing*, 38, 713–747, 2016.

[3] D. Balzani, D. Böse, D. Brands, R. Erbel, A. Klawonn, O. Rheinbach and J. Schröder. Parallel Simulation of Patient-specific Atherosclerotic Arteries for the Enhancement of Intravascular Ultrasound Diagnostics. *Engineering Computations*, 29, 2012.

[4] D. Balzani, P. Neff, J. Schröder, G. Holzapfel, A polyconvex framework for soft biological tissues. Adjustment to experimental data. *International Journal of Solids and Structures*, 43, 6052–6070, 2006.

Modeling of active response of arteries

R. Gilbert (TU Clausthal), S. Hartmann (TU Clausthal), L. Kudela (TU München), E. Rank (TU München), O. Yossef (Ben-Gurion University of the Negev), Z. Yosibash (Ben-Gurion University of the Negev) 16:50

Even though many studies have been conducted to understand and model the passive response of arteries, very few studies have been performed to develop the constitutive equation for active response of arteries. In our investigation, a small length of porcine artery is used to perform, as a first step, tension-inflation experiments for the passive response. Afterwards, norepinephrine is added to activate the smooth muscle cells in the artery. The experiment is kept as close to in-vivo conditions as possible. A special testing device has been developed for applying axial displacements, internal pressure and norepinephrine, and to measure both the axial force as well as the radial deformation by means of digital images.

In this presentation, a constitutive model considering the passive and active response is chosen for media and adventitia. A common carotid porcine artery is harvested and equilibrated for one hour and then tension-inflation followed by activation of the arteries with norepinephrine is performed. In arteries, the norepinephrine diffuses into the artery through the intima and into the media. The smooth muscle cells in the media contracts accordingly to the concentration of the norepinephrine. The same concept is used to model the active response of the arteries. The mechanical response is coupled with the diffusion equation. To find the best-fit parameters in a least square sense, a trust region reflective algorithm, provided in Matlab is used. An optimization data tool has been developed, which calls the FEM program during each iteration of the optimizer. Finally, the total response of the simulated model is compared to the experimental results.

Development of patient-specific computational models of the human aortic valve under healthy and diseased conditions

S. Morales (Universität Stuttgart), O. Röhrle (Universität Stuttgart) 17:10

For investigating the cause-effect factors that link the destructive remodelling processes of an aortic valve's extracellular matrix (ECM) with ventricular diseases, it is essential to efficiently construct patient -specific 3-d Finite Element models of human aortic valves. Under the assumption that the function, deformation and performance of the valve is strongly dependent on the valvular geometry, we first focus on the model generation of the valves. For this purpose, a series of valvular geometries is extracted from medical imaging data (MRI, 3D-TEE and CT) to replicate patient-specific human aortic valve's geometry. The geometry encompasses the asymmetry and regional thicknesses. Both influence the biomechanical behaviour of the valve. Moreover, suitable constitutive models for the valves are derived from experimental data as well as from literature. Further, case-specific boundary conditions are applied to the models to reproduce the bending and tensile stretches suffered by the cusps along the heart cycle. The overall aim of this project is to use modelling to determine for a range of ventricular and aortic pressure loading patterns the resulting stress and strains distributions within the aortic cusps. The loads are assumed to be ranging from typical pressures occurring in healthy

left ventricles to pressures that occur in left ventricles exhibiting different stages and types of cardiomypathy. By comparing the stress and deformation patterns computed from the models with the patterns of calcification incidence as well as with the dynamics of the valves observed in medical imaging data, we can generate useful data to study the development of calcific aortic valve disease from initial alterations in the tissue to end-stage calcification.

Analysis and Optimization of Inlet and Outlet Boundary Conditions for Flow Simulations in Circle of Willis

A. Alimi (University of Kassel), O. Wünsch (University of Kassel) 17:30

Blood flow simulation of complex arterial networks in three-dimensions generally involves assigning many inlets and outlets. This work involves study of different kind of boundary conditions assigned on multiple inlets as well as the outlets in Circle of Willis. Circle of Willis is a circle consisting of different arteries supplying the brain blood with multiple bifurcations, where the conservation of mass would be applied. Considering the complex geometry of Circle of Willis, there are arteries with different shapes either flowing inward or flowing outward the circle [1]. Generally, there are multiple small vessels and capillaries in each artery. Hence, to reduce the complexity of the geometry and simulations of blood flow, these small arteries and capillaries could be truncated. Truncating the arteries in downstream of the arterial trees needs assigning an appropriate boundary condition on the truncation points. These points are in general bounded using outflow boundary conditions. There are different type of suitable models to simulate the pulse wave in the arteries such as resistance model or impedance model [2][3]. Although predefined pressure profile could be a good choice for the inlets of the circle, outflow boundary conditions can affect the wave velocity profile in the upstream arteries. These conditions have to be implemented in a way that the assumption of periodic blood pressure and periodic flow rate are both satisfied. In this work, inlet and outlet boundary conditions will be adopted in a way that a realistic velocity profile and pressure in the main brain arteries are achieved for a transient blood flow [4]. The 3D model and its grid generation are done using ANSYS® 17.1, while the numerical simulations would be performed by *OpenFOAM®*.

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[2] T. Du, D. Hu, and D. Cai: Outflow Boundary Conditions for Blood Flow in Arterial Trees. PLoS One, 10 (5): e0128597. doi:10.1371/journal.pone.0128597, (2015)

[3] L. Grinberg, G. E. Karnidakis: Outflow Boundary Conditions for Arterial Networks with Multiple Outlets. Annals of Biomedical Engineering, Vol. 36, No. 9, pp. 1496-1514, (2008)

[4] J. R. Womersley: Method for the calculation of velocity, rate of flow and viscous drag in arteries when the pressure gradient is known. J. Physiol. 127, 553-563, (1955)

Emergence of aortic aneurysms due to failure of adhesive bonds between proteoglycans

M. Hillgärtner (Department of Continuum Mechanics, RWTH Aachen University), K. Linka (Department of Continuum Mechanics, RWTH Aachen University), M. Itskov (Department of Continuum Mechanics, RWTH Aachen University) 17:50

Aortic aneurysms are a common disease among older patients. Aneurysm ruptures cause more than 150 000 deaths annually [2]. One of the main risk factors which lead to the abnormal enlargements of vessels (>150% of original size) is arterial hypertension.
This contribution presents a modeling approach, where the cyclic loading of the artery caused by the blood pressure leads to fatigue inside the arterial wall. The arterial wall is considered as a composite material, where a matrix (ground substance) is reinforced by collagen fibers consisting of fibrils connected by proteoglycan (PG) bridges. These PG bridges support interfibrillar sliding, which leads to the lower fibril stretch [4]. Molecular adhesive bonds rupture under any pulling force if the force is held sufficiently long enough [1]. This rupturing over time leads to a decrease in the density of PG bridges, higher stretches in the fibrils, more damage inside the fibrils and finally to fatigue of the soft tissue which causes the abnormal enlargement. Finally, the model is compared against experimental data of uni-axial tension tests and used in a FEM simulation to study the emergence of aortic aneurysms under arterial hypertension.

[1] E. Evans, K. Ritchie (1997). Dynamic strength of molecular adhesion bonds. Biophysical Journal, 72(4), 1541-1555.

[2] Global Burden of Disease Study (2015). Global, regional, and national age-sex specific all-cause and cause-specific mortality for 240 causes of death, 1990-2013: a systematic analysis for the Global Burden of Disease Study 2013. Lancet, 385(9963), 117-171.

[3] K. Linka, V. N. Khiêm and M. Itskov (2016). Multi-scale modeling of soft fibrous tissues based on proteoglycan mechanics. Journal of Biomechanics, 49, 2349-2357.

[4] S. Rigozzi, R. Müller, A. Stemmer and J.G. Snedeker (2013) Tendon glycosaminoglycan proteoglycan sidechains promote collagen fibril sliding-AFM observations at the nanoscale. Journal of Biomechanics, 46, 813-818.

Method for the Development of Realistic Boundary Condition for the Simulation of Non-Contact Tonometry

S. Münch (Dresden Center for Computational Materials Science DCMS, TU Dresden), D. Balzani (Institute of Mechanics and Shell Structures, TU Dresden), M. Röllig (Fraunhofer Institute for Ceramic Technologies and Systems IKTS), E. Spörl (Universitätsklinikum Carl Gustav Carus, TU Dresden) 18:10

In industrialized countries a high number of glaucoma disease are not diagnosed, because in the early stages there seems to be no symptoms. Without an early diagnosis, glaucoma lead to significant impairments, for example a limitation of the visual field. In the year 2012 972.000 people were affected by these impairments in Germany [1]. The method of treatment is only based on eye surgery, which could be avoided by an early diagnosis. Today the measurement of the Intraocular Pressure (IOP) is the state-of-the-art diagnosis for glaucoma, but just fifty percent of glaucoma patients have an increased IOP. Because that is not satisfying, a new diagnosis technique is needed. A measurement of the biomechanical properties of the transparent front part of the eye, called cornea, is promising. Many numerical simulations have been considered to extract these properties from in vivo examinations with non-contact tonometer like the Corvis® ST, which records the eye deformation during an air pulse non-invasively. But an essential question is unexplained: which boundary condition gives a realistic imitation of the air pulse? We propose a method based on combining a specific experiment with numerical calculations to identify the time-dependent pressure distribution. We use a glass eye suspended on a yarn and positioned in front of the Corvis® ST nozzle exit. At the backside of the eye, a laser triangulation sensor is used to measure the time dependent movement of the glass eye during the air pulse. These data are derived to the acceleration time curve and multiplied with the weight of the glass eye to obtain the force operating on the eye. Then, a numerically stable computational fluid dynamic (CFD) model of the glass eye in front of the nozzle is built. Afterwards, simulations with different pressure amplitudes at the nozzle inlet were performed to determine the force on the eye resulting from the inlet pressure. In the next step we inversely calibrate the inlet pressure with the forces extracted from the pendulum experiment. The calibrated model is then used to extract the time-dependent pressure distribution on the cornea surface.

[1] Wolfram C, Pfeiffer N. Weißbuch zur Situation der ophthalmologischen Versorgung in Deutschland. Deutsche Ophthalmologische Gesellschaft, München. 2012

S 2 : Biomechanics

Thursday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 101
Chair: Markus Böl (TU Braunschweig)

A study of the performance of a posterior dynamic stabilisation device using numerical simulation and experimental data

A. Beckmann (RWTH Aachen University), M. Stoffel (RWTH Aachen University), B. Markert (RWTH Aachen University) 14:00

Rigid posterior fixation devices are the golden standard for treatment of degenerative lumbar stenosis associated with spinal instability. In the last decades, plenty of new posterior dynamic stabilisation devices (PDSD) were developed to gain the aimed stabilisation by maintaining the physiological kinematics of the spine. The PDSD are loaded dynamically in the body, have to be made of biocompatible material, and need to have a considerable flexibility. Besides these sophisticated design requirements, it is a known problem of PDSD to undergo fatigue failure.

The aim of this study is to predict the fatigue failure of a PDSD through comparison of a 3D finite element (FE) simulation with experimental data. To this end, a 3D FE model of a PDSD, which showed fatigue failure in an on-going clinical study, was created using μCT data. Experiments were carried out to obtain material parameters of the PDSD. The PDSD was included in a modified FE model of the lumbar spine, which was developed and validated in a former study [1]. Experimental results of the instrumented spine of a former in vitro study were compared to the simulated results. The fatigue behaviour of the PDSD was estimated with varied load modes using principal stresses of the computation model and published data of fatigue behaviour of the materials.

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Biomechanical Evaluation of a Femoral Neck Fracture Implant using a Novel Test-Stand

M. Mundt (Institute of General Mechanics), S. Bettag (Department of Orthopedic Trauma Surgery), F. Bamer (Institute of General Mechanics), M. Stoffel (Institute of General Mechanics), M. Knobe (Department of Orthopedic Trauma Surgery), B. Markert (Institute of General Mechanics) 14:20

The application of endoprotheses in the treatment of femoral neck fractures shows promising results. However, in some cases it is advantageous to apply head-conserving implants. The Rotation-stable Screw Anchor (RoSA) is mounted to increase the stability of this specific type of femoral neck injury by its innovative screw-blade design. Nonetheless, it is not clear if the use of cement as an additional fixation of the implant improves the stability of the biomechanical system [1].

In order to investigate and compare the stability of the implants, human cadaver femora

are tested in a novel test-rig. Hereby, on the one side of a femur pair a cemented implant and on the other side a cement-free implant is attached. For reliable testing, a novel test-rig, which is able to imitate gait cycles, is developed. The time-dependent force applied to the bone is based on an in vivo study of Bergmann et al. [2]. Two hydraulic cylinders of a material testing machine (Mini Bionix 858, MTS, Eden Prairie, MN, USA) are used to load the bone in axial and lateral direction. The motion of each of the three segments, screw, femur head and femur shaft, is recorded by an optical infra-red camera system (Nexonar, soft2tec GmbH, Rüsselsheim, Germany). Hereby, virtual markers are used to determine the motion of the specific measurement points. The applied load is based on the mean body weight of an elderly person (main patient group). Four loading conditions are considered according to the statistically estimated weights of the patients [3]. After the cyclic loading procedure, the bone is loaded to failure by a linearly increasing force. Using the time-dependent force and position information different parameters of the biomechanical system are evaluated and compared statistically.

[1] Dr. K. Maier: RoSA Rotationsstabiler Schraubanker - ein innovatives Fixationsprinzip des Kopf-Hals-Fragmentes bei Frakturen am coxalen Femurende (2011), `http://www.koenigsee-implantate.de/specials/rosa_de.php`, 08/12/2016.
[2] Bergmann, G., Deuretzbacher, G., Heller, Graichen, F., Rohlmann, A., Strauss, J., Duda, G.N. (2001). Hip contact forces and gait patterns from routine activities. Journal of Biomechanics, 34, 859-871.
[3] requested at DESTATIS Statistisches Bundesamt in May 2016.

Vibration of the Basilar Membrane in the Human Inner Ear

P. Ziegler (University of Stuttgart), P. Wahl (University of Stuttgart), P. Eberhard (University of Stuttgart) 14:40

The inner ear or cochlea is a bone structure of spiral shape and is composed of mainly two conical chambers which are filled with fluid and separated by a soft membrane, the basilar membrane. At the apical end, both chambers are connected to each other through a small opening, called the helicotrema. At the base, the chambers are closed by the stapes footplate and the round window membrane. The cochlea can, therefore, be considered as a closed hydraulic system. Sound is received by the eardrum, transmitted through the middle ear ossicles and finally excites the inner ear fluid through the vibration of the stapes footplate. This leads to pressure waves in the cochlear fluid which in turn results in characteristic vibration behavior of the basilar membrane. Related to the sound frequency, hair cells in certain areas of the basilar membrane are stimulated and cause hearing nerve stimulation.

To investigate this system, a coupled Finite Element model with acoustic elements is presented. With this model, it can be shown that the position of the maximum amplitude of the basilar membrane depends on the excitation frequency at the oval window. For low frequencies, the position of the maximum amplitude is located closer to the apex, while for high excitation frequencies the maximum is situated closer to the base. Additionally, the frequency distribution along the length of the basilar membrane as well as the impact of fluid viscosity on the basilar membrane vibration are investigated. Then, the pressure

distributions along the length of the two fluid-filled chambers are evaluated to investigate the interaction between fluid pressure and motion of the basilar membrane. These results provide a deeper understanding of the formation of the characteristic vibration of the basilar membrane.

Three-dimensional analyses of dental reconstructions with the Finite-Element-Method

P. Joedecke (Hochschule Magdeburg-Stendal), C. Weber (Hochschule Magdeburg-Stendal) 15:00

In analyzing and evaluating the behavior of organic structures researchers in all disciplines are throughout confronted by the following question: How should the level of detail be chosen? We have been investigating this and other questions in the field of dental reconstruction for several years using the FEM (Finite-Element-Method). Special attention was paid to the use of anatomical structures (dentin, enamel, pulp, periodontal ligament) from radiological data. These were calculated for complex models (upper and lower jaw) including tooth stock. By validating the calculated / theoretical values with in-vitro examinations, the complete workflow can be carried out from the creation of a CAD model to the production, including subsequent quality control.

Personalized simulations of tibial fractures during gait

M. Roland (Universität des Saarlandes), B. Braun (Universität des Saarlandes), R. Derr (Universität des Saarlandes), T. Pohlemann (Universität des Saarlandes), S. Diebels (Universität des Saarlandes) 15:20

When fractures heal the tissues involved in the healing process respond to the mechanical signals introduced through loading of the fracture. Theoretically the right amount of stress allowed by the osteosynthesis and introduced through load bearing promotes healing, while either over- or underloading will result in healing delay and eventually non-union. Therefore, an insole based pedobarography is used to monitor the patient postoperative weight bearing during fracture healing. To simulate the biomechanical aspects of this process and the healing outcome, finite element models are designed with respect to the patient-specific fracture morphology and the individual weight bearing behavior to compute the resulting interfragmentary strains. The fracture morphology data was obtained both from X-ray images and from computed tomography image stacks. In the case of 2D X-ray images, the computer models are generated by using a CAD software solution and material classes close to the mechanical properties of bone and soft tissue. For the case of 3D tomogram information, the following workflow was used: segmentation of the image stack, assignment of the material information by converting CT data given in Hounsfield units to mechanical properties and meshing via a hexahedral topology. Both biomechanical simulation concepts are used in this study and compared against one another. In addition, the results from the monitoring data driven simulations are compared with results using the OrthoLoad database as gait input data. The results of these personalized patient-specific simulations can be used as a decision support system for medical health professional analyzing the healing outcome.

Optimal Hip Implant Positioning

M. Moldenhauer (Zuse Institute), M. Weiser (Zuse Institute) 15:40

In an aging society where the number of joint replacements rise, it is important to also increase the longevity of implants. In particular hip implants have a life-time of at most 15 years. This derives primarily from pain due to migration, wear, inflammation, and dislocation, which is affected by the positioning of the implant during the surgery. Current joint replacement practice uses 2D software tools and the experience of surgeons. Especially the 2D tools fail to take the patients natural range of motion as well as stress distribution in the 3D joint induced by different daily motions into account. Optimizing the hip joint implant position for all possible parametrized motions under the constraint of a dynamic contact problem is prohibitively expensive as there are too many motions and every position change demands a recalculation of the contact problem. For the reduction of the computational effort, we use adaptive refinement on the parameter domain coupled with the interpolation method of Kriging. A coarse initial grid is to be locally refined using goal-oriented error estimation, reducing locally high variances. This approach will be combined with multi-grid optimization such that numerical errors are reduced.

S 2 : Biomechanics

Thursday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 101
Chair: Udo Nackenhorst (Leibniz Universität Hannover)

The influence of binder mobility to the viral entry driven by the receptor diffusion

S. Klinge (TU Dortmund University), W. Tillmann (TU Dortmund University), G. Holzapfel (TU Graz), R. Gilbert (University of Delaware) 16:30

The current presentation deals with the simulation of the viral entry into a cell. There are two dominant mechanisms typical of this process: the endocytosis und the fusion with the cellular membrane. However, we only focus on the first scenario. To this end, we consider a virus as a substrate with a constant concentration of receptors on the surface. Differently, the concentration of receptors of the host cell varies and these receptors are free to move over the membrane. When the contact with the cell surface has been achieved, the receptors start to diffuse to the contact (adhesion) zone. The membrane in this zone inflects and forms an envelope around the surface of the virus. This is the way the newly formed vesicle imports its cargo into the cell. In order to simulate the process described, we assume that the differential equation typical of the heat transport is suitable to simulate the diffusion of receptors. Additionally, we formulate two boundary conditions: First, we consider the balance of fluxes on the front of the adhesion zone. Here, it is supposed that the velocity is proportional to the gradient of the chemical potential. The second subsidiary condition is the energy balance equation depending

on four different contributions: the energy of binding receptors, the free energy of the membrane, the energy due to the curvature of the membrane and the kinetic energy due to the motion of the front. The differential equation itself along with two boundary conditions forms a well-posed problem which can be solved by applying a direct method, for example the finite difference method. The talk also includes numerical examples showing the distribution of receptors over the membrane as well as the motion of the front of the adhesion surface. In particular, the influence of the mobility of receptors has been studied.

Estimation of Transpiration Rate in Herbaceous Plants Using Theory of Porous Media

P. Asgharzadeh (Universität Stuttgart), A. Birkhold (Universität Stuttgart), O. Röhrle (Universität Stuttgart) 16:50

Determination of water exchange in an ecological system such as areas covered by various types of plants to predict growth and survival of the ecological system is of major interest in establishing silvicultural plans. In this study, by means of a finite element simulation of the stem of a herbaceous plant, the transpiration rate and influx of water through the roots based on acquired material properties and geometry through experimental data are determined based on the theory of porous media. To do so, a dynamic simulation of a biphasic porous medium is utilized to determine the pressure profile and the displacement of the stem, caused by the flow and pressure profile through a 24 hours simulation time. The result is an estimation of transpiration rate and influx of the system that can reproduce the experimental data from pressure probes inside the stem and video recordings of the movement of the stem during 24 hours. Due to the simplicity of the proposed method and the ease of gathering input data, the deformation of the system, this FE simulation can be an alternative to the more common approach of measuring CO_2 consumption of plants in a closed environment for the purpose of quantifying water exchange.

Energetic aspects in the modelling of frost-resistant plant tissues

L. Eurich (Institute of Applied Mechanics (CE), University of Stuttgart), A. Wagner (University of Stuttgart), W. Ehlers (University of Stuttgart) 17:10

Plant tissues have developed several strategies to sustain temperatures below the freezing point without any frost damage. Some of these strategies are of physiological nature, others arise from structural properties. Here, the focus is on the structural properties of plant tissues. A key mechanism is the dehydration of the cell body, as freezing within the cells is a critical process threatening the structural integrity and even the ability of a plant to survive. Thus, the water leaves the cell body and flows within the vascular bundles to preferred locations (ice lensing), where freezing is not assumed to be critical. This indicates that the controlled flow management capability is a further important mechanism, which is mainly determined by structural properties of the cell bodies.

This implies that frost-resistant plant tissues can be understood as porous materials,

as they are formed by cells with intra- and extracellular spaces. A sound multicomponent and multiphasic continuum-mechanical model is realised within the Theory of Porous Media (TPM), where processes on the microscale are related to a homogenised macroscopic model. This is achieved by a volumetric homogenisation of the microscopic structure within a representative elementary volume (REV), resulting in superimposed and interacting constituents. In terms of frost-resistant plant tissues four constituents are considered in the model. In particular, the model proceeds from a thermoelastic solid skeleton (formed by the cell bodies) containing initially trapped water. Within the pore space, two mobile fluids are present, namely materially compressible air and materially incompressible water, where the latter can be subjected to a phase transition and turns into ice, which is then kinematically coupled to the motion of the solid skeleton.

The above mentioned mechanisms are described in case of the cell dehydration by a production term in the mass balance of the solid skeleton accounting for the fact that with decreasing temperature the water is no longer trapped within the cell body. The flow management capability is described by anisotropic permeability conditions. The freezing process of the pore water is characterised by a density jump at the interface and the coexistence of both phases during the freezing process. The interface is conceptionally treated by a singular surface, at which a mass transfer can be formulated with the help of jump conditions. Furthermore, the phase change of the pore water from a liquid state of aggregation to a solid one leads to the necessity to consider the so-called compaction point in the material description, accounting for the case that there is no pore space present anymore. The resulting system of coupled partial differential equations is solved numerically using the in-house developed Finite-Element (FE) environment PANDAS. The presented numerical examples illustrate the behaviour of frost-resistant plant tissues under freezing conditions and show, in particular, the anisotropic perfusion and the freezing of the accumulated cell water towards preferred locations.

Optimal Geometry of Compliant Pressure Actuated Cellular Structures

M. Pagitz (University of Stuttgart), R. Leine (University of Stuttgart) 17:30

The multifunctionality and relative simplicity of plant cells is fascinating. Unlike humans and animals, plants do not possess a centralized skeleton and complex control system. Yet they can create their own food through photosynthesis, reproduce, carry considerable external loads and in some cases are even capable of rapid movements. The nastic movement of plants is caused by cell pressure variations of up to 5 MPa that require a water flow between neighboring cells. Skotheim and Mahadevan found that the speed of plant movements increases for decreasing cell sizes and pumping distances. Hence it is best if water fluxes occur mainly between neighboring cell layers. Based on these observations Pagitz et al developed a novel concept for adaptive structures. This concept is based on rows of prismatic pentagonal and hexagonal cells. The geometry of each cell can be optimized such that a cellular structure with n_R cell rows deforms into n_R target shapes for given cell row pressures. Compliant pressure actuated cellular structures can undergo large shape changes while being strong and lightweight. Hence their potential application ranges from passenger seats to leading and trailing edges of aircraft.

The difficulty in realizing this concept lies in the optimization of cell geometries for given target shapes and cell pressures. Directly optimizing the cell geometries is impractical since it requires a detailed two-dimensional continuum finite element model. Instead, a lower-dimensional numerical model is optimized in a first step. In the numerical model, each cell side is replaced by axial and rotational springs with hinge eccentricities. The stiffness constants and eccentricities depend on the geometry of the continuum model. This reduction is possible due to a concentration of bending strains in regions around cell corners. Such a numerical model for the shape optimization of compliant pressure actuated cellular structures has been previously published by the authors. The current contribution enhances the numerical framework by introducing the associated continuum model. The side lengths of the numerical model can be optimized for given stiffness constants and eccentricities such that the equilibrium shapes for given cell row pressures are identical to the target shapes. However, the resulting geometry of the associated continuum model may then be awkward or even impossible to construct. Furthermore, the maximum hinge and cell side stresses in the continuum model may be far from optimal. Hence it is necessary to solve a fully coupled problem such that the structure both meets the target shapes and has a proper geometry. It is shown that the computation of optimal cell corner geometries within the continuum model requires a bilevel optimization approach. Furthermore, it is shown how the continuum and numerical model are fully coupled. A further benefit of this approach is that the optimized continuum model can be directly sent to a rapid prototyping machine. Several examples are used to demonstrate the performance of the proposed approach.

Analytical treatment of autonomous and heteronomous boundary-value problems in context of bio-inspired tactile object sensing

C. Will (TU Ilmenau, Fak. Maschinenbau), J. Steigenberger (TU Ilmenau/ Fak. MN), C. Behn (TU Ilmenau, Fak. Maschinenbau) 17:50

Rodents like rats exhibit different types of tactile hairs. A special type is represented by the so-called mystacial vibrissae. They are located around the snout and each vibrissa is supported by its own follicle-sinus complex which serves as a measurement unit. The hair with this follicle can be seen as a powerful tactile sensor. With them, these animals are able to detect the distance to an object, recognize the object shape, and determine the surface texture. Here, the focus is on object shape recognition. For this, a model of a technical vibrissa is set up which shall adapt similar properties and features of the paragon. The vibrissa is modeled as an Euler-Bernoulli bending beam without linearization. The object scanning procedure consists of a single-sweep of an one-sided clamped beam from the right to the left along an object, assuming the object profile's boundary being a strictly convex function and having an ideal contact with the beam. This mechanical model is described by a set of first-order, nonlinear differential equations with boundary conditions and unknown parameters: a two-point boundary-value problem which is not necessarily autonomous when focussing on tapered or pre-curved vibrissae. An analytical treatment of the mathematical problem in dealing with standard elliptic

integrals results in a decision criterion for a phase distinction (tip contact or tangential contact of beam with object) and a development of an object shape reconstruction algorithm, just based on the determined (and later measured in experiments) observables an animal solely relies on: the support reactions.

Influence of Vibrissa morphology on Artificial Tactile Sensors for Surface Texture Detection

M. Scharff (TU Ilmenau, Fak. Maschinenbau), J. Steigenberger (TU Ilmenau/ Fak. MN), C. Behn (TU Ilmenau, Fak. Maschinenbau) 18:10

Animals, e.g., rats and cats, have different types of tactile hairs. One type are the mystacial vibrissae. They are located around the snout and in combination with the follicle-sinus complex they are powerful tactile sensors. With them, animals are able to detect the distance to an object, recognize the object shape and determine the surface texture. Adapting the natural example, the goal is to design an artificial tactile sensor with a similar functionality. In the course of this, a model for surface texture detection is developed. The vibrissa is modeled as an Euler-Bernoulli bending beam, incorporating large deflections. The contact, between vibrissa and surface, is modeled using Coulomb's law of Friction. The mechanical modeling results in a nonlinear, heteronomous, system of first order differential equations. Solving the boundary-value problem by applying a shooting method, a quasi-static simulation is performed. Some first relations between the vibrissa morphology and the surface contact are analyzed. With view to an artificial sensor, the change of the reaction forces and moments at the base of the vibrissa due to the surface contact is the point of focus. Out of the reaction forces, the coefficient of static friction between vibrissa and surface is determined.

S 3: Damage and fracture mechanics

Organizers: Martin Hofmann (TU Dresden, Institut für Festkörpermechanik)
Andreas Ricoeur (University of Kassel)

S 3 : Damage and fracture mechanics

Tuesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 106

Determination of the diameter of columnar jointed volcanics using bifurcation analysis

R. Anderssohn (TU Dresden, Institut für Festkörpermechanik), M. Hofmann (TU Dresden, Institut für Festkörpermechanik) 14:00

The development of the columns with the typical hexagonal pattern of solidifying volcanic material can be described by fracture mechanics. While following the moving inhomogeneous temperature field, the columns reach a steady growth. During this growth

the columns evolve a relatively constant diameter, which happens to be always close to the point of bifurcating to an increased crack spacing by leaving segments of the crack front behind. Knowing the fracture toughness of the material and the velocity of the temperature field, the crack spacing and the geometry of the bifurcation mode is predicted by an equilibrium analysis based on the free Helmholtz energy. The number of necessary first and second partial derivatives of the energy is minimized by approximating the crack front with a Fourier series expansion. The derivatives are calculated with the Finite Difference method. The free Helmholtz energy is computed via a linear elastic and three-dimensional Finite Element simulation. Incorporating the symmetries of an idealized hexagonal pattern reduces the size of the FE model.

Asymptotic analysis of notch induced crack nucleation

J. Felger (Technische Universität Darmstadt), W. Becker (Technische Universität Darmstadt) 14:20

In the presence of geometrical or material discontinuities in elastic structures, the corresponding stress field possesses singularities at which mathematically infinite stresses occur. Such points of highly localised stress concentration typically represent the location of failure initiation represented by the onset of cracks within the framework of brittle fracture. If the length of the initiating crack is small compared to a characteristic structural length, methods of asymptotic analysis can be applied very advantageously giving a physical insight into the fracture mechanics problem and allowing for a significant reduction of the required numerical effort performing a fracture mechanics analysis.
In the present study, a semi-analytical asymptotic approach is used in order to analyse the effect of crack initiation at a sharp re-entrant corner on the change of total potential energy and the field quantities of the elastic body. The elastic fields in the unperturbed (uncracked) configuration are described using a complex potential approach [1]. Based on the work by Leguillon [2, 3, 4], a matched asymptotic expansion procedure using two different scales is established leading to semi-analytical relations involving the crack length explicitly. The construction of higher order terms at the inner and outer level of the asymptotic expansions is discussed in detail and their influence on the solution behaviour is thoroughly examined. Furthermore, full-numerical analyses are performed in order to quantify the accuracy of the asymptotic solutions and their validity range. It it shown that higher order terms allow for identifying a specific length induced by the underlying asymptotic assumptions, characterising the scale of admissible crack lengths.

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Crack path predictions in anisotropic structures considering residual stresses

P. Judt (University of Kassel), A. Ricoeur (University of Kassel) 14:40

Different mechanical processes induce a directional microstructure (texture) during the production of a material, e.g. during the hot rolling of aluminum plates or the injection molding process of natural fiber reinforced bio-polymers. In such materials the anisotropic mechanical features are related to the texture and have a decisive impact on the fracture process. Rolling or shot peening processes induce an irreversible plastic deformation and residual compressive stresses for the purpose of a surface toughening. Similarly, residual stresses are induced if a circular core with interference fit is inserted into a drilled hole.

This work focuses on he anisotropy of the elastic and fracture mechanical material properties and to residual stresses due to a core. In case of numerical crack tip loading analyses and the simulation of crack paths, these features must be taken into account. An efficient method for the accurate calculation of crack tip loading quantities in a FE-framework are path independent integrals, such as J_k- and interaction-integrals [1, 2]. Utilizing their path-independence, essentially reliable numerical data far from the crack tip are exploited. Special treatment is necessary if large integration contours are considered and curved crack faces [3], internal boundaries, material interfaces or inelastic effects within the integration region are considered. This approach is suitable for the accurate prediction of crack paths in structures with orthotropic fracture toughness [4]. The measurement of crack paths in specimens with residual stresses due to a core reveals an influence of the core's interference with respect to the crack deflection and the resulting paths [5, 6]. Numerical investigations show that conventional crack deflection criteria are not valid in such specimens, as the deflection angle depends on the external loading, going along with a rotation of the principal stress axes and the J_k-vector [6]. A new criterion considering the rotation of the J_k-vector is presented and numerical crack paths are calculated and compared with experiments.

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Simulation of crack growth under mixed-mode loading in 1D quasicrystals

Z. Wang, A. Ricoeur (University of Kassel) 15:00

Lacking translational symmetry in particular directions, quasicrystals (QC) are a new class of materials besides crystals and amorphous solids, where 1D means in one direction the atomic arrangement is quasiperiodic. Since the very first discovery in 1982, QC have been the focus of theoretical and experimental studies in the physics of condensed matter [1, 2]. The investigation of physical properties of quasicrystals, such as the fracture behaviour, electronic properties and hardness etc., is essential extending their fields of application. Today, QC are known to exhibit e.g. a very good wear resistance, low friction coefficients and to possess a very low porosity. However, the fracture behavior of QC is not clear yet. This work presents a generalized fracture theory including the J-integral and crack closure integrals as well as the implementation of the near-tip solution in 1D QC. Some fracture criteria are generalized for quasicrystals and compared [3]. Numerical tools and a re-meshing algorithm have been developed to simulate crack growth under mixed-mode loading.The energy-based criterion predicts that there may be a substantial impact of phonon-phason coupling on the crack deflection angle. The simulation shows that the crack path depends strongly on the quasi axis. The influence of the new introduced phason field in QC on crack deflection is discussed.

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Time-harmonic analysis of cracks in functionally graded piezoelectric materials

M. Wünsche (Slovak Academy of Sciences), J. Sladek (Slovak Academy of Sciences), V. Sladek (Slovak Academy of Sciences), C. Zhang (University of Siegen) 15:20

Keywords: piezoelectric FGMs, time-harmonic loading, crack analysis, BEM

Modern piezoelectric structures offer certain performance advantages over conventional ones due to their capability of converting electrical energy into mechanical energy and vice versa. In recent years composites with a continuously change of the material properties are getting increasing attention in advanced engineering applications. An important advantage over conventional laminates is that interfaces and stress discontinuities are avoided. Piezoelectric composites are very brittle and have a low fracture toughness [1]. The analysis of functionally graded materials (FGMs) is mathematically complex and analytical solutions are possible only for very simple geometry and loading conditions. Therefore, efficient numerical methods are needed to solve more general problems.
In this paper, time-harmonic crack analysis in two-dimensional piezoelectric FGMs is presented. For this purpose, a frequency-domain boundary element method (BEM) is developed [2]. Since fundamental solutions for piezoelectric FGMs are not available, a boundary-domain integral formulation is derived. This requires time-harmonic fundamental solutions for homogeneous piezoelectric materials. The radial integration method is adopted to compute the resulting domain integrals. Adjacent the crack-tips square-root elements are implemented to capture the local square-root-behavior of the generalized crack-opening-displacements properly. Numerical examples will be presented and discussed to show the influences of the material gradation, poling direction and the dynamic loadings on the intensity factors.
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S 3 : Damage and fracture mechanics

Tuesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 106

Experimental investigation and numerical simulation of fatigue crack formation in polycrystalline materials

J. Hohe (Fraunhofer-Institut für Werkstoffmechanik IWM), C. Beckmann 16:30
(Fraunhofer-Institut für Werkstoffmechanik IWM), T. Kennerknecht
(Fraunhofer-Institut für Werkstoffmechanik IWM), J. Preußner
(Fraunhofer-Institut für Werkstoffmechanik IWM), M. Farajian
(Fraunhofer-Institut für Werkstoffmechanik IWM), M. Luke
(Fraunhofer-Institut für Werkstoffmechanik IWM)

Fatigue crack initiation under cyclic loading is a major concern in structural application. For characterization of the crack formation phase, a combined experimental and numerical investigation on the microscale is performed. The experimental investigation is based

on micro specimens with gauge sections in the range of 200 µm x 450 µm taken from the heat affected zone of a ferritic weldment. The specimens are fatigued in a special customized micromechanical test rig and investigated with respect to their microstructure prior to and after the experiments. By this means, a direct correlation between microstructure, local loading conditions and the risk of fatigue crack formation is established. The experimental investigation is complemented by a microscopic numerical simulation using a multi-grain volume element in conjunction with a homogenization analysis. Employing a stochastic simulation strategy, the probability distributions for the cycles necessary for formation of a prescribed microcrack can be determined. The numerical predictions are found in a good agreement with the experimental observations.

Investigations on dynamic fracture of ultra-high performance concrete by Brazilian tests

M. Khosravani (University of Siegen, Chair of Solid Mechanics,), K. Weinberg (University of Siegen, Chair of Solid Mechanics,) 16:50

In the last years significant advances in energy-absorption capabilities of concrete and concrete-like materials have been made and a new generation of concrete has been introduced. Greatly improved microstructure compared to traditional concrete, led to production of Ultra-high performance concrete (UHPC) which shows improved material properties and higher performance. Despite of many potential applications, specific technical information about this material is still limited. This research presents a linear elastic fracture mechanic based model which is used to study fracture behavior and some mechanical fracture parameters of UHPC material. In a series of test, flattened and original Brazilian disc specimens are impacted by a split Hopkinson pressure bar (SHPB). Dynamic properties such as the dynamic E-modulus and fracture toughness are calculated by an experimental-numerical method. As two different groups of the UHPC specimens are tested, the effects of specimen geometry on dynamic fracture is also found. On the experimental setup, original complete Brazilian discs and also flattened Brazilian specimens are tested. Data acquisition system recorded the strain history during the experiment by the help of strain gauges which are mounted on the incident and transmission bars and on the specimens. Moreover, numerical fracture analysis is conducted and good agreement between theory and experiments is observed. The achieved results prove that the Brazilian test is a powerful and efficient method to study dynamic fracture properties of UHPC material.

Characterization of radial cracks emanating from boreholes using X-Ray computed microtomography

D. Uribe (University of Stuttgart), Y. Cheng (Ruhr Universität Bochum), J. Renner (Ruhr Universität Bochum), H. Steeb (University of Stuttgart) 17:10

Hydraulic fracturing of rocks is an important process for several industrial applications like oil and gas reservoir stimulation, hydrothermal energy production, and CO_2 sequestration. Comparing the mathematical models that describe the process of hydraulic fracturing still present challenges to predict the direction in which a crack propagates,

the breakout pressure, the initiation of multiple fractures at the borehole wall and the hydro-fracturing process using viscous fluids[1, 2]. One of the processes which still require further study is the initiation of the fracture in the borehole from hydraulic stimulation, i.e. raising the borehole-fluid pressure to the breakdown pressure.
To gain new insight into the fracture mechanism, we hydro-fractured rock cores from the same material with different borehole diameters. After fracturing, the boreholes were filled with epoxy and smaller cores are drilled around the borehole to aid tomographic acquisition. Using X-Ray micro Computed Tomography (XRCT)[3], the volumetric data of the fractured boreholes was obtained. After image filtering and segmentation, the borehole and fracture surface points were isolated. Further post processing of the surface points involved the fitting of parametric surfaces. Finally, from the parameters of the fitted surfaces, we were able to identify some of the theoretical mismatches present in the literature. We discuss the possible reasons for these mismatches from the measurements done on the parametric surfaces together with the information gathered during hydraulic stimulation.

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Effects of Process Parameters on Interlaminar Fracture Toughness of Consolidated Glass Fiber Reinforced Polyamide-6 Tapes

M. Schober (Karlsruhe Institute of Technology (KIT)), T. Kuboki (The University of Western Ontario), E. Ameri (The University of Western Ontario), J. Hohe (Fraunhofer Institut für Werkstoffmechanik (IWM)), P. Gumbsch (Karlsruhe Institute of Technology (KIT)) 17:30

Consolidated continuous fiber reinforced thermoplastic tapes have recently been used for light-weight structural parts as well as light-weight patching material to locally reinforce a specific part area. The manufacturing process of consolidated tapes consists of three steps: tape laying, heating, and compression of the tape layers. Whereas the tape laying process allows arbitrary shapes and stacking sequences, the consolidation process merges the individual tape layers and thus provides structural integrity of the lay-up. It is important to understand how this manufacturing method affects microstructures at the interface and mechanical properties, in particular, fracture toughness between the tape layers. In this study, unidirectional, glass fiber reinforced polyamide-6 tapes are manufactured using industry-scale process equipment: an automated tape laying machine, a

convection oven, and a hydraulic press. Consolidated tapes are prepared under different consolidation temperatures and pressures. The consolidated tapes' interlaminar fracture toughness is evaluated using the double cantilever beam (DCB) tests for Mode I, the end notched flexure (ENF) test for Mode II, and the mixed-mode bending (MMB) test for mixed Modes I and II. Based on the results, the effects of the process conditions on the interlaminar fracture toughness of the consolidated tapes are discussed.

S 3 : Damage and fracture mechanics

Wednesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 106

3D Fracture modeling by extended finite element method and gradient enhanced damage

M. Pezeshki (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), S. Löhnert (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 14:00

In this research crack growth in brittle media is investigated by means of the eXtended Finite Element Method (XFEM) and damage mechanics. An essential advantage of the XFEM is that the finite element mesh does not require updating to be able to track the crack path [1]. To track the advancing crack location at each increment within the considered domain correctly and accurately, the Level Set Method was employed. Level Sets obtained based on the signed-distance functions are updated by using a geometrical approach only in the vicinities of the advancing crack fronts. The corrected XFEM approach with the first branch function is utilized here [2]. In the corrected XFEM formulation, a global enrichment function is localized by the multiplication by a ramp function resolving problems in the blending elements.

An isotropic gradient enhanced damage model is utilized to evaluate degradation of the material at each point of the domain. In gradient enhanced damage models, a chosen length scale behaves as a localization limiter and describes the influence of the microstructure on the damage process [3]. Moreover, such a model smoothes the deformation of the structure and avoids energy dissipation in a narrow band as well as mesh dependency. The damage value at the crack front in each time increment is found and compared with a critical value which is the criterion for crack propagation.

To find the crack propagation direction, these two methods are considered: maximum circumferential (hoop) stress and the gradient of the damage field. In the first method, the values of hoop stress in a predefined distance along an arc around each point of the crack front is examined to find a maximum value [4]. Then the crack is propagated along this direction. In the second method, the gradient of the damage field along the crack

front line is considered to find the propagation direction. Finally the results of the two methods are compared.

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A model for coupled inelastic deformation and anisotropic damage behaviour of concrete

A. Monnamitheen Abdul Gafoor (Institut für Statik, TU Braunschweig), 14:20
D. Dinkler (Institut für Statik, TU Braunschweig)

A great range of efforts has been taken for the development of continuum damage models to describe the deformation behaviour of brittle materials as concrete. Even though, isotropic damage models are considered for a first approximation, they may lead to noticeable errors in real applications. Since the micro-cracking of concrete occurs due to sequential application of directional loads, the damage in concrete has to be anisotropic for a reliable representation of damage.

Initially an isotropic damage model based on energy equivalence is developed. The model adopts a damage evolution law similar to Weibull's failure distribution [1]. The damage evolution is driven by damage equivalent strain using a single loading surface for tension and compression due to Lubliner failure criterion [2]. Thus, the model is capable of describing different behaviour of concrete in tension and in compression. The numerical results exhibit good agreement with experimental results [3, 4].

Nevertheless, the direction of damage growth under multi-axial loading conditions is undefined so far in the model. Thus, the previous model is extended to capture the direction of possible damage evolution. The measure of damage is split-up into two measures of damage, namely tensorial anisotropic damage due to deviatoric state of stress and isotropic damage due to hydrostatic state of stress. The damage evolution in anisotropy depends on the growth of principal strain in corresponding directions. In case of isotropic damage, it depends on the damage equivalent strain defined earlier.

In addition, the damage initiation is different in tension and compression behaviour of concrete accordingly.
Further investigations under cyclic loadings show its inability of capturing residual strains compared to experiments [4]. Thus, the present proposal of work includes the coupling of inelastic behaviour of material in the extended anisotropic damage model and the verification of proposed model.

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A gradient-extended damage-plasticity model to counteract mesh-dependence in finite element simulations

T. Brepols (Institute of Applied Mechanics, RWTH Aachen University), S. Wulfinghoff (Institute of Applied Mechanics, RWTH Aachen University), S. Reese (Institute of Applied Mechanics, RWTH Aachen University) 14:40

The understanding and prediction of damage and fracture processes in elastoplastic structures have ever since been topics of major interest in the scientific field of computational mechanics. From a microstructural point of view, void nucleation, growth and coalescence are the predominant physical mechanisms leading to ultimate failure in ductile materials. In continuum damage mechanics (CDM), these individual phenomena are usually modeled by means of one (or several) internal damage variables which account for the aforementioned microstructural defects in an averaged sense. Even though CDM is nowadays well-accepted as a suitable framework to describe progressing damage at a macro continuum level, the specific type of constitutive description of combined plasticity and damage, the interplay between the two phenomena during evolving failure as well as their concurrent algorithmic treatment in numerical simulations all remain subjects of intensive debate in the literature and lead to ongoing research in the community (among many others, see e. g. [1]). Another topic attracting particular attention is related to suitable regularization techniques avoiding pathological mesh-dependence in finite element simulations involving conventional 'local' CDM models, rendering corresponding results often useless for meaningful subsequent analyses (see e. g. [2]).
Against this backdrop, a specific gradient-extended damage-plasticity model is discussed which is based on the micromorphic approach in the spirit of Forest [3, 4]. Plasticity and damage are modeled using a two-surface formulation in which both are considered as separate physical mechanisms which, however, strongly influence each other. The

existence of separate loading / unloading conditions and corresponding multipliers for plasticity and damage complicates the algorithmic treatment and necessiates further considerations which are explained in detail. Various numerical benchmark simulations are performed and discussed in order to assess the respective properties of the material model and carefully examine its potential to regularize finite element simulations involving elastoplastic material behavior with softening.

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3D ductile crack propagation within a polycrystalline microstructure using the XFEM and a nonlocal damage model

S. Loehnert (Leibniz Universität Hannover), S. Beese (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 15:00

During forming processes of steels within the polycrystalline microstructure cracks might nucleate and propagate and eventually lead to the failure of the material. In addition, during the time the formed engineering part is in service, the damage development emanating from the production of the part might have an influence on its lifetime. Hence, it is important to know about the initiation and growth of microcracks and their effect on the macroscopic behaviour of the material and the engineering part.

In this contribution we present a method to calculate crack propagation within the polycrystalline microstructure of steels under finite deformations. The method incorporates the XFEM in combination with level set techniques and a nonlocal Gurson type damage model in combination with finite deformation crystal plasticity. The nonlocal damage can be interpreted as a void volume fraction, and its value along the crack front is used to determine whether the discrete part of the crack propagates. We define the crack propagation direction as the direction of fastest void volume growth. For details of this approach we refer to [1].

Due to complicated crack geometries and crack propagation the XFEM enrichments of nodes might lead to badly conditioned global system matrices due to possible near linear dependencies between standard and enriched degrees of freedom or between enriched degrees of freedom. This problem has been addressed in [2] and other publications. One way to overcome this problem is to stabilize the element stiffness matrices by adding some small artificial stiffness to those eigenmodes that should not have a nearly zero eigenvalue. This technique is presented for the case of linear elastic fracture mechanics in [2]. Here it is extended and applied to the severely nonlinear case including localization phenomena.

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[2] S. Loehnert: A stabilization technique for the regularization of nearly singular extended finite elements. *Computational Mechanics*, vol 54, pp 523 – 533, (2014)

Implementation of a dissipation based path-following method and its application to the simulation of nonlocal quasi-brittle damage

S. Prüger (TU Dresden, Professur für Mechanik und Flächentragwerke), 15:20
D. Balzani (Institute of Mechanics and Shell Structures, TU Dresden, and Dresden Center for Computational Materials Science (DCMS))

Many natural materials, e.g. ice and marble and man-made materials such as concrete show a brittle or quasi-brittle damage behavior. This characteristic material behavior results in severe nonlinearities and convergence issues when the response of structural components and their degradation needs to be simulated. In this case, well-known snap-through or snap-back responses are observed, which led to the development of path-following techniques, c.f. [1, 2]. These techniques augment the system of nonlinear equations, which result from the finite element discretization of the boundary value problem by an additional load-scaling parameter and an associated constraint equation for the path length. In the incremental-iterative procedure normally employed in the solution of the systems of nonlinear equations, the regular force or displacement control is abandoned and the solution is sought simultaneously for the displacement and the load-scaling parameter. Recently, a competitive path-following technique has been proposed in [3], which formulates the constraint equation for the path length in terms of the dissipation increment in the structure. Originally the dissipation increment is obtained by a simple explicit integration of the dissipation. Here, we propose an alternative formulation based on a more stable implicit integration of the dissipation and address the issue resulting from this specific choice of integration procedure, namely the incorporation of the derivative of the consistent tangent w.r.t. the displacements in the linearization of the constraint equation. This path-following technique is then applied to simulate one-dimensional quasi-brittle damage, for which an integral averaging is

employed to obtain mesh-independent results.

[1] Crisfield, M.A., "A fast incremental-iterative solution procedure that handles snap-through",*Computers & Structures*, 13, pp. 55-62, 1981

[2] Ritto-Correta, M., Camotim, D., "On the arc-length and other quadratic control methods: Established, less known and new implementation procedures", *Computers & Structures*, 86, pp.1353-1368, 2008

[3] Verhoosel, C.V., Remmers, J.J.C., Gutierrez, M.A.,"A dissipation-based arc-length method for robust simulation of brittle and ductile failure", *International Journal for Numerical Methods in Engineering*, 77(9), pp.1290-1321, 2009

Calibration of a gradient-enhanced damage model for viscoplastic shell structures subjected to shock-wave loadings

A. Nguyen (RWTH-Aachen University), M. Stoffel (RWTH-Aachen University) 15:40

The main goal of our study was to establish both a numerical and experimental methodology for material parameter identification to validate the gradient-damage model in [1,2,3]. For this purpose, micro-bending and -tensile tests were conducted to identify the physical damage length scales. Furthermore, an experimental procedure was established to determine the gradient parameters and to validate the proposed model. For numerical simulation, the model in [2] was extended to analyse the anisotropic nonlocal damage of the plates and shells as additional efforts to generalise for the case of anisotropic damage. In more general terms, our study wanted to investigate how the damage length scales effect on the vibration of the plates subjected to shock-waved loading. The softening behaviour by taking into account the weighting of the nonlocal effects was of our interests. Ten micro-tensile tests for copper specimens of 20-40 μm thicknesses and 36 micro-bending tests for ones of 25-40 μm are conducted. The first is used to identify the parameters for the damage and viscoplastic evolution including kinematic hardening effects, while the latter to identify the nonlocal damage parameters for the proposed enhanced free energy function.

[1] A. D. Nguyen, M. Stoffel, *DFG Final report STO 469/6-2* (2015).
[2] A. D. Nguyen, M. Stoffel, and D. Weichert , A gradient-enhanced damage approach for viscoplastic thin-shell structures subjected to shock waves. *Comp. Meth. App. Mech. Engrng.*, 217-220, 236–246 (2012).
[3] M. Stoffel (2007). An experimental method for validating mechanical models. *Mechanik Berichte Nr.5*, RWTH Aachen University.

S 3 : Damage and fracture mechanics

Wednesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 106

A phase field approach to fracture coupled with mass transport for the simulation of environmentally-assisted damage

R. Falkenberg (BAM Federal Institute for Materials Research and Testing) 16:30

With the introduction of a mass transport mechanism the entire problem is subjected to a time frame that dictates the time-dependent action of soluted species on mechanical properties. A numerical framework within the phase field approach is presented with an embrittlement-based coupling mechanism. The underlying functionals are expressed in terms of the displacement, the mass concentration and the crack phase field. Within the phase field approach the modeling of sharp crack discontinuities is replaced by a diffusive crack model facilitating crack initiation and complex crack topologies without the requirement of a predefined crack path. The isotropic hardening of the elasto-plastic deformation model and the local fracture criterion are affected by the species concentration. This allows for embrittlement and leads to an accelerated crack propagation. An extended mass transport equation for hydrogen embrittlement, accounting for mechanical stresses and deformations, is implemented. For stabilisation purposes a staggered scheme is applied to solve the system of partial differential equations by a multi-field finite-element method. A thermodynamically consistent coupling relation that accommodates the required mechanisms is presented.

Phase-field modeling of ductile fracture processes

F. Streich (Institut of Mechanics, Karlsruhe Institute of Technology (KIT)), M. Dittmann (Chair of Computational Mechanics, University of Siegen), C. Hesch (Chair of Computational Mechanics, University of Siegen) 16:50

Phase-field methods to fracture problems have draw a lot of attention throughout the past years, since they allow for convenient and efficient simulation of complex fracture pattern. Several limitations of various phase-field models are currently under investigation. In particular, fracture at finite strains (see [1]) along with ductile and cohesive fracture problems are subject to extensive research. Moreover, higher-order finite deformation phase-field formulations (see [2]) can be implemented in a straight-forward manner using quadratic NURBS basis functions.

In this talk, we aim at a elasto-plastic formulation for ductile fracture problems by combining gradient plasticity with the phase-field approach. Therefore, we introduce new concepts for the inevitable anisotropic split of the strain energy in tension and compression.

Several examples will demonstrate the applicability of the proposed formulations in two and three dimensions. A higher-order phase-field approach using Cahn-Hilliard like approximation of the phase-field along with hierarchical refinement procedures allows for

an efficient computational treatment within a finite element framework. A detailed analysis of the incorporation of inelastic effects will be shown.

[1] C. Hesch and K. Weinberg, Thermodynamically consistent algorithms for a finite-deformation phase-field approach to fracture, *Int. J. Numer. Meth. Engng.*, 99:906–924, 2014.

[2] C. Hesch, M. Franke, M. Dittmann and İ. Temize, Hierarchical NURBS and a higher-order phase-field approach to fracture for finite-deformation contact problems, *Computer Methods in Applied Mechanics and Engineering*, 301:242–258, 2016.

Neural network representation of a phase-field model for brittle fracture

A. Koeppe (RWTH Aachen University), F. Bamer (RWTH Aachen University), C. Hernandez Padilla (RWTH Aachen University), B. Markert (RWTH Aachen University) 17:10

Phase-field models constitute a powerful tool in fracture mechanics. However, the main issues of these type of methods are the selection of phase-field parameters, as well as the requirements of very finely meshed structures and extremely small integration time steps. The subject of this work is the construction of an artificial neural network representing a finite element model coupled with a phenomenological phase-field approach for brittle fracture. The resulting neural network [1] can rapidly predict the behavior of the phase-field model with trained, internal parameters. The approach is demonstrated on a plate with a hole in 2D. The neural network results and computation time is compared to established phase-field models [2].

[1] A. Koeppe, F. Bamer, and B. Markert. Model reduction and submodelling using neural networks. *PAMM*, 16(1):537–538, Oct. 2016. ISSN 1617-7061. doi: 10.1002/pamm.201610257.

[2] S. P. Patil, Y. Heider, C. A. Hernandez Padilla, E. R. Cruz-Chú, and B. Markert. A comparative molecular dynamics-phase-field modeling approach to brittle fracture. *Computer Methods in Applied Mechanics and Engineering*, 312:117–129, Dec. 2016. ISSN 0045-7825. doi: 10.1016/j.cma.2016.04.005.

Variational framework for phase field modeling of ductile fracture in porous solids at finite strains

S. Teichtmeister (University of Stuttgart), D. Kienle (University of Stuttgart), F. Aldakheel (University of Stuttgart), C. Miehe (University of Stuttgart) 17:30

This work outlines a rigorous variational-based framework for the phase field modeling of fracture in isotropic and anisotropic porous solids undergoing large elastic-plastic deformations. It extends the recent work [1] to a formulation of porous plasticity with

particulate microstructures characterized by spherical pores or by ellipsoidal voids, which undergo a change in size and orientation.
The phase field approach regularizes sharp crack surfaces within a pure continuum setting by a specific gradient damage modeling with geometric features rooted in fracture mechanics. A gradient plasticity model for isotropic and anisotropic porous plasticity with a simple evolution law for the void volume fraction is developed, and linked to a failure criterion in terms of the local elastic-plastic work density that drives the fracture phase field [2]. It is shown that this approach is able to model phenomena of ductile failure such as cup-cone failure surfaces. On the side of damage mechanics only two material parameters are needed, namely a critical work density that triggers the onset of damage and a shape parameter that governs the postcritical damage up to fracture.
The coupling of gradient plasticity to gradient damage is realized by a constitutive work density function that includes the stored elastic energy and the dissipated work due to plasticity and fracture. With this viewpoint at hand, the thermodynamic formulation is outlined for gradient-extended dissipative solids with generalized internal variables.
The proposed canonical theory is shown to be governed by a rate-type minimization principle, which describes the coupled multifield evolution problem of plasticity-damage, where on the side of plasticity an additive split of the total Hencky strain is used.
A further aspect of this work is the regularization towards a micromorphic gradient plasticity-damage setting by taking into account additional internal variable fields linked to the original ones by penalty terms. This enhances the robustness and facilitates the finite element implementation, in particular on the side of gradient plasticity.

[1] C. Miehe, S. Teichtmeister and F. Aldakheel. Phase-field modelling of ductile fracture: a variational gradient-extended plasticity-damage theory and its micromorphic regularization. *Philos T Roy Soc A*, 374, 2015.

[2] C. Miehe, D. Kienle, F. Aldakheel and S. Teichtmeister. Phase field modeling of fracture in porous plasticity: A variational gradient-extended Eulerian framework for the macroscopic analysis of ductile failure. *Comput Method in Appl M*, 312:3–50, 2016.

Phase-Field Modelling of Fracture - Formulation, Adaptivity and Applications

M. Kästner (TU Dresden, Institut für Festkörpermechanik), P. Hennig (TU Dresden, Institut für Festkörpermechanik), T. Linse (TU Dresden, Institut für Festkörpermechanik), C. Bilgen (Universität Siegen, Lehrstuhl für Festkörpermechanik), M. Dittmann (Universität Siegen, Lehrstuhl für Numerische Mechanik), C. Hesch (Universität Siegen, Lehrstuhl für Numerische Mechanik), K. Weinberg (Universität Siegen, Lehrstuhl für Festkörpermechanik) 17:50

The phase-field method has become a powerful tool for the modelling of fracture [1].

Its essential idea is to smear the discrete crack in terms of a crack density which is used as phase-field order parameter. Due to the diffuse representation of the crack, topological updates of the analysis mesh are avoided which is particularly helpful for the analysis of crack branching and three-dimensional problems. The versatility of the approach comes, however, at the cost of highly refined meshes that have to resolve strong gradients across the internal characteristic length scale ℓ_0. Therefore, adaptive local refinement is essential to the successful application of the approach.
At first, we review different phase-field models of fracture, e.g. second- and fourth-order models as well as various conditions to ensure irreversibility of crack growth, and compare the resulting physical behaviour. In particular we discuss the requirement that for $\ell_0 \to 0$, the smeared crack Γ_{ℓ_0} has to converge to the discrete crack Γ. We extend our previous findings on the influence of boundary conditions and the finite size of specimens [3] and critically discuss the assumptions that are necessary to apply the phase-field approach to brittle fracture.
Motivated by the findings of the numerical analysis, we apply multi-level hierarchical splines [2], i.e. a sequence of nested uniformly h-refined B-splines or NURBS which provide efficient and locally refinable discretisations for both – second- and fourth-order phase-field models. We have developed procedures for adaptive local refinement based on Bézier extraction [4] which enable the incorporation of the approach into existing finite element codes and avoid the explicit generation of the hierarchical basis. It is found that the adaptively refined meshes produce the same force-displacement curves but significantly reduce the number of used elements and the required computation time when compared to uniform mesh refinement.
Eventually, the performance and efficiency of the adaptive refinement are examined for different applications in phase-field modelling of fracture, e.g. problems of small and finite deformations, fracture in homogeneous and heterogeneous materials, and the modelling of interface cracks.

Acknowledgements:
The present project is supported by the German Research Foundation (DFG) within the Priority Programme (SPP) 1748. This support is gratefully acknowledged.

[1] B. Bourdin, G. Francfort, J.-J. Marigo, Numerical experiments in revisited brittle fracture. *MECH PHYS SOLIDS* **48** (2000) 797–826.

[2] C. Hesch, S. Schuß, M. Dittmann, M. Franke, K. Weinberg. Isogeometric analysis and hierarchical refinement for higher-order pahse-field models. *COMPUT METHOD APPL M* **303** (2016) 185-207.

[3] M. Kästner, P. Hennig, T. Linse, V. Ulbricht, Phase-Field Modelling of Damage and Fracture—Convergence and Local Mesh Refinement. In: *Advanced Methods of Continuum Mechanics for Materials and Structures*, Springer (2016) 307-324.

[4] P. Hennig, S. Müller, M. Kästner, Bézier extraction and adaptive refinement of truncated hierarchical NURBS. *COMPUT METHOD APPL M* **305** (2016) 316-339.

A Phase Field Model for Ductile Fracture under Thermomechanical Loadings

Z. Liu (Otto-von-Guericke Universität Magdeburg), D. Juhre (Otto-von-Guericke Universität Magdeburg) 18:10

The phase field method has emerged as an extremely powerful technique to simulate crack initiation and propagation with significant success [1]. Phase-field-type diffusive crack approach is capable of predicting the crack initiation and propagation without any additional criterion [2, 3]. Here, its main advantages are the ability to predict crack initiation and to handle curved crack paths, crack kinking, branching angles and crack-front segmentation in three dimensions [5, 5]. The study of fracture under thermomechanical loadings is a numerically difficult topic since temperature is treated as an additional degree of freedom. The aim of this contribution is to propose a new generalized phase field model for ductile fracture in elasto-plastic solids under thermomechanical loadings. Therefore, the recently proposed phase field formulation by Ambati et al. [6] has been extended to predict damage initiation and propagation of a ductile material exhibiting J_2-plasticity due to thermomechanical loadings. Several benchmark tests of crack nucleation and propagation analyses in elasto-plastic materials under thermomechanical loadings are carried out. The results demonstrate the performance of the proposed phase field model for ductile fracture under thermomechanical loadings.

[1] M. Ambati, T. Gerasimov, L. De Lorenzis. A review on phase-field models of brittle fracture and a new fast hybrid formulation. Computational Mechanics, 55, 383–405, 2014.

[2] C. Kuhn, R. Müller. A continuum phase field model for fracture. Engineering Fracture Mechanics, 77, 3625–3634, 2010.

[3] C. Miehe, M. Hofacker, F. Welschinger. A phase field model for rate-independent crack propagation: robust algorithmic implementation based on operator splits. Computer Methods in Applied Mechanics and Engineering, 199, 2765–2778, 2010.

[4] C. Miehe, F. Welschinger, M. Hofacker. Thermodynamically consistent phase-field models of fracture: Variational principles and multi-field FE implementations. International Journal for Numerical Methods in Engineering, 83(10), 1273–1311, 2010.

[5] C. Miehe, S. Teichtmeister, F. Aldakheel. Phase-field modelling of ductile fracture: A variational gradient-extended plasticity-damage theory and its micromorphic regularization. Philosophical Transactions of the Royal Society of London A, 374, 1–18, 2016.

[6] M. Ambati, T. Gerasimov, L. De Lorenzis. Phase-field modeling of ductile fracture. Computational Mechanics, 55, 1017–1040, 2015.

S 3 : Damage and fracture mechanics

Thursday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 106

Application and parameter identification of cohesive zone elements for intergranular fracture in thin layers

S. Rezaei (Institut für Angewandte Mechanik), S. Wulfinghoff (Institut für Angewandte Mechanik), S. Reese (Institut für Angewandte Mechanik) 14:00

Coating layers are usually applied on different manufacturing tools to improve their wear resistance and surface properties of the final parts [1]. In this work, fracture and damage behavior of hard coatings such as (Cr,Al)N is studied. The intergranular fracture within the coating system is modeled by employing cohesive zone (CZ) regions at grain boundaries. The coatings are produced by means of direct current magnetron sputtering (dcMS) and the high power pulsed magnetron sputtering (HPPMS) method. The elasto-plastic properties of the coating as well as their morphology were measured based on nanoindentation tests and scanning electron microscope (SEM) measurement, respectively [2]. In order to perform a bending test, at first, the coating layer is isolated from the substrate in form of a cantilever beam. The fracture properties of the coating are measured by investigating the force-displacement curve obtained from the bending test. The cohesive zone element parameters are then fitted to the experimental results to simulate the same behavior. Based on the measured parameters, more simulations such as nanoindentation tests with geometrically more complex interfaces are performed. The influence of the mechanical properties of different components in a coating system on the damage and crack propagation are investigated in detail. Similar crack patterns were observed comparing the numerical and experimental results in nanoindentation test.

The influence of strong and weak interfaces on crack propagation in plane elastic structures

J. Scheel (University of Kassel), A. Ricoeur (University of Kassel) 14:20

The improvement of properties or functional applications are the reason for inserting any kind of inclusion in an otherwise homogeneous material. These inclusions exhibit interfaces having an influence on propagating matrix cracks. The interfaces can either be strong or weak, where a suitable model has to be applied for possible delamination. Cohesive zone models are a good possibility to do so. It is experimentally proven that a matrix crack tends to grow towards regions with lower stiffness [1,2], so that delamination cracks in the interface might be attractive for matrix cracks too. The purpose of this research is to simulate the matrix crack growth in bi-material structures, incorporating dissipative processes arising at weak interfaces and to provide a reference by simulating the crack propagation in the same bi-material but with a strong (perfect) interface. The matrix crack growth is simulated by incremental crack extensions, leading to a continuous modification of the geometry. Intelligent re-meshing is therefore required, where the loading history cannot be neglected [3]. In order to determine the crack tip loading and

crack deflection, the J-integral and stress intensity factors, respectively, are calculated . The simulations indicate, that the matrix crack tends to grow into the direction of regions with lower stiffness. In the case of weak interfaces, the delamination has an extremely attracting effect on propagating matrix cracks, which is stronger than the influence of soft or stiff domains. The distance from the matrix crack to the interface also determines the extent of deflection.

[1] Tilbrook, M. T., Rozenburg, K., Steffler, E. D., Rutgers, L., and Hoffman, M.: Crack propagation paths in layered, graded composites. *Composites Part B: Engineering 37* (2006), 490–498.
[2] Judt, P. O., Ricoeur, A., and Linek, G.: Crack path prediction in rolled aluminum plates with fracture toughness orthotropy and experimental validation. *Engineering Fracture Mechanics 138* (2015).
[3] Judt, P. O. and Ricoeur, A.: Quasi-static simulation of crack growth in elastic materials considering internal boundaries and interfaces. *Key Engineering Materials, 525* (2013), 181-184.

Fatigue Damage and Degradation Model for Carbon Fibre Reinforced Polymer Materials

Z. Abdul Hamid (Karlsruhe Institute of Technology (KIT)), J. Hohe (Fraunhofer Institute for Mechanics of Materials IWM), M. Gall (Fraunhofer Institute for Mechanics of Materials IWM), S. Fliegener (Fraunhofer Institute for Mechanics of Materials IWM), P. Gumbsch (Karlsruhe Institute of Technology (KIT)) 14:40

A major issue concerning Carbon Fibre Reinforced Polymer (CFRP) materials under cyclic loading is that the materials often undergo material degradation starting from the initial stage of the loading. For a laminate that consists of different fibre orientation plies, this becomes crucial as it causes redistribution of stresses and strains during the lifetime of the component. Understanding the importance of a reliable fatigue damage and degradation model in the development of reliability assessment of CFRP materials, the present studies contribute to this by considering the effect on a single-ply material level, exclusively under fatigue loading. The model is developed based on a modified Hooke's Law to account for the typical anisotropic damage of the material. It considers three independent damage variables in 3 individual spatial directions, i.e. the direction of fibres, and both lateral directions. It is restricted to be applied to stiff and brittle materials with characteristic properties similar to those of carbon-epoxy composites. The model is implemented through a user subroutine into a commercial Finite Element program (Abaqus) and applied to a database of uniaxial fatigue experiments. The model is found to be able to accurately predict the degradation and failure of the CFRP composite materials under fatigue loading.

A continuum model for intralaminar damage progression and delamination in layered composites

J. Simon (RWTH Aachen University), D. Höwer (RWTH Aachen University), S. Reese (RWTH Aachen University), J. Fish (Columbia University) 15:00

Carbon fiber reinforced composites have become very popular in numerous applications in aerospace, automotive, and maritime industry. They are typically composed of either unidirectional carbon fibers or textiles, in which the reinforcing fibers are woven or braided, embedded in an epoxy matrix material. These composites are advantageous due to their ease of manufacture, damage tolerance, and relatively low cost.
However, physics-based modeling of their mechanical behavior is challenging. While in the unidirectional case all fibers are considered as perfectly aligned in one particular direction, textile composites introduce additional geometric complexities, which cause significant local stress and strain concentrations. Since these internal concentrations are primary drivers of nonlinearity, damage, and failure within textile composites, they must be taken into account in order for the models to be predictive.
In this paper, an anisotropic continuum damage model is presented, which enables accounting for the interaction of damage evolution in different directions by introducing six independent damage variables. The model is thermodynamically consistent and mesh independent due to use of an energy based regularization scheme.
It is shown that the model can be successfully applied on different scales: on the micro-scale of unidirectional CFRP it is applied in an isotropic manner for the matrix material, whereas on the meso-scale of textile composites the same model can be used to describe the orthotropic damage behavior of the yarns. Moreover, on the macro-scale the model allows the prediction of delamination in layered composites.

Micromechanical Damage Modeling of Long Fiber Reinforced Composites with the Parametric High Fidelity Generalized Method of Cells

M. Schmerbauch (Kassel University), A. Levi-Sasson (Tel-Aviv University), J. Aboudi (Tel-Aviv University), A. Matzenmiller (Kassel University), R. Haj-Ali (Tel-Aviv University), F. Erler (Kassel University) 15:20

Micromechanical damage modeling of long fiber reinforced composites is presented by using both continuum and interface damage mechanics at the constituents levels. The two damage approaches have been separately implemented with the parametric high fidelity generalized method of cells (HFGMC). This well-established micromechanical method is used to solve the fine-scale boundary value problem for the spatial variants of the local fields, as well as to predict the effective mechanical behavior of periodic composite materials. The HFGMC utilizes a repeating unit cell (RUC) to represent the microstructure, enforcing in an integral average the continuity and periodicity of tractions and displacements along the subcell boundaries in the RUC, as well as the static equilibrium of each subcell. For the interface damage approach, traction-separation of two adjacent subcells along their common interface is taken into account by replacing the

displacement continuity through an interfacial jump condition. This modeling technique enables the representation of fiber and matrix cracking as well as fiber-matrix debonding. On the other hand, the continuum damage approach describes evolving damage within the material phases of the composite. The growing strain-softening damage influences the microscopic fields and, thus, the effective mechanical behavior of the composites. The damage and stress distribution predicted by the two approaches are compared within the RUC under remote uniaxial stress loading. In addition, failure envelopes are created based on the prediction of the effective stress-strain response, and compared with the forecast of Puck's macromechanical fracture model.

Shear cutting of fiber reinforced plastics

L. Poggenpohl (Institute of Applied Mechanics, RWTH Aachen University) 15:40

In this project, the punching process of carbon fiber reinforced plastic (CFRP) is investigated numerically and experimentally. Punching presents a low cost and potentially high quality manufacturing technology for piercing, but has not been investigated sufficiently so far for CFRP.
The numerical part of the project aims on the key mechanical processes from a damaging point of view. Therefore methods of damage and/or fracture mechanics are used. Experiments are executed to get the material parameters and to investigate crack growth within the material. The macro scale simulations will be supported by micro scale investigations.
The goal of the project is to identify the principle influence parameters on the quality of the cutting face from a simulational and an experimental point of view.

S 3 : Damage and fracture mechanics

Thursday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 106

LATIN approach for fatigue damage computation

S. Alameddin (IBNM, Leibniz Universität Hannover), M. Bhattacharyya (IBNM, Leibniz Universität Hannover), A. Fau (IBNM, Leibniz Universität Hannover), U. Nackenhorst (IBNM, Leibniz Universität Hannover), D. Néron (LMT, ENS Cachan, CNRS, Université Paris Saclay), P. Ladevèze (LMT, ENS Cachan, CNRS, Université Paris Saclay) 16:30

Non-linear mechanical behaviour such as (visco)plasticity or damage is generally tackled with time incremental methods where the time domain is subdivided into incremental steps. Then a numerical scheme is carried out consequently for each time step. In contrast, in LArge Time INcrement (LATIN) method [1], an approximation of the total time history process is sought directly. This is done by an iterative sequence of two steps:

tackling the global linear mechanical equilibrium equation on one side, and on the other one the local history process is determined. The global stage can benefit from model reduction techniques such as the proper generalised decomposition (PGD), in order to obtain a substantial reduction of the computational cost. Moreover, for parametric problems, efficient reduced models can easily be derived.
The LATIN method has been well established to compute several types of problems including material non-linearities [2] but has not been extended to unilateral damage law which leads to a non-linear state equation. An extension of the method is then introduced herein to tackle this issue and then to benefit from a promising numerical framework for fatigue damage computation.

[1] P. Ladevèze, *Nonlinear computational structural mechanics: new approaches and non-incremental methods of calculation*. New York, NY: Springer New York, 1999.

[2] P. Ladevèze, "On reduced models in nonlinear solid mechanics," *European Journal of Mechanics - A/Solids*, vol. 60, pp. 227 - 237, 2016.

Molecular dynamics simulations of the cooling rate influence on the fracture behaviour in silica glasses

F. Ebrahem (RWTH Aachen University), S. Patil, B. Markert (RWTH Aachen University) 16:50

In the present work, we focused on the understanding of the atomistic fracture behaviour of amorphous silica by means of molecular dynamics (MD) simulations. Here, we used a two-body and a three-body interaction potential [1] to generate various amorphous states by quenching molten SiO_2. This quenching process was carried out for different cooling rates [2]. Finally, tensile tests were performed on amorphous silica until fracture, and the cooling rate influence on the energy release rate was analysed using Griffith's theory [3]. Our analysis paves the way towards the multiscale modelling of amorphous silica.

[1] Vashishta, P., Kalia, R.K., Rino, J.P., Ebbsjö, I.: *Interaction potential for SiO_2: A molecular-dynamics study of structural correlations*, Vol. 41 of Physical Review B. American Physical Society, pp.12197–12209 (1990).
[2] Chowdhury, S.C., Haque, B.Z., Gillespie, J.W.: *Molecular dynamics simulations of the structure and mechanical properties of silica glass using ReaxFF*, Vol. 51 of Journal of Materials Science. Springer, pp.10139-10159 (2016).
[3] Griffith, A.A.: *The phenomena of rupture and flow in solids*, Vol. 221 of Philosophical Transactions of the Royal Society of London. Series A, Containing Papers of a Mathematical or Physical Character. JSTOR, pp.163–198 (1921).

Analysis of Hertzian indentation fracture in the framework of finite fracture mechanics

M. Strobl, P. Dowgiallo, T. Seelig (Karlsruher Institut für Technologie (KIT)) 17:10

Fracture initiation at the defect-free surface of a brittle solid subjected to indentation loading has experimentally been investigated already by H. Hertz more than a century ago, e.g. [1], but resists a complete theoretical description by classical fracture mechanics still to date. While classical fracture mechanics relies on the pre-existence of a well-defined crack, the concept of finite fracture mechanics assumes the *spontaneous formation* of a finite crack, e.g. [2], and therefore is a promising tool to study problems as the one mentioned above.

In the present work, indentation fracture initiation is analyzed in the framework of finite fracture mechanics which requires the simultaneous fulfillment of a stress based and an energetic criterion. A semi-analytical and a numerical evaluation of the energetic criterion are investigated, and the functionality of the hybrid criterion in application to indentation fracture is discussed in detail. Moreover, the predictive capabilities are illustrated by comparison with experimental results from the literature [3].

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Modeling of damage behavior and size effect of interphase in polymer - nanocomposites using micropolar continuum theory

S. Ma (Institute of General Mechanics, RWTH Aachen University), B. Markert (Institute of General Mechanics, RWTH Aachen University) 17:30

Adding nanoparticles into polymer matrix leads to significant improvements of mechanical properties in terms of stiffness, strength and toughness. Due to physical and chemical interactions between the nanoparticles and the matrix, a thin layer with graded properties referred to as interphase forms between them during manufacturing process of nanocomposites. At the nanoscale, the dimensions and volume fraction of the interphase are comparable with those of reinforcement and matrix. The interphase highly affects the loading transfer mechanisms and mechanical behavior of the nanocomposites. In order to improve the understanding of the role of inhomogeneous interphase on the inelastic deformation and damage behavior of the nanocomposites, a proper constitutive model of the nanostructured interphase is required for the computational investigation of the structure-property relationship.

In the present work, a constitutive model based on the micropolar theory is proposed for modeling the inelastic deformation and damage behavior of inhomogeneous inter-

phase. The size-effect and graded material properties of interphase are directly taken into account in the formulation of constitutive model. An inverse method using FE simulations is applied to calibrate the mechanical and physical properties of interphase using experimental data. Furthermore, the effect of the gradient structure of interphase on the reinforcement performance of nanocomposites is analyzed based on micromechanical models.

Key words:
Micropolar continuum theory; inhomogeneous interphase; damage modeling; nanocomposites

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The coupling of plasticity with a relaxation-based approach to damage modeling

S. Schwarz (Institute of Mechanics of Materials, Ruhr-Universität Bochum), P. Junker (Institute of Continuum Mechanics, Ruhr-Universität Bochum), K. Hackl (Institute of Mechanics of Materials, Ruhr-Universität Bochum) 17:50

Since damage occurs in context of high stresses which are also related to the development of plastic strains, it is natural to couple damage and plasticity phenomena to achieve a more realistic model. Hereto, the new damage model presented in [1] was used and enhanced with plasticity and isotropic hardening. Thereby, the damage model is based on a new regularization approach and provides mesh independent results. In order to achieve mesh independency, damage models usually take into account the non-local behavior by using a field function which couples the local damage parameter to a non-local level, in which differences between the local and non-local parameter as well as the gradient of the non-local parameter can be penalized [1]. In contrast, the new regularization approach no longer needs a non-local level at the finite element scale but directly provides mesh-independent results. Due to the new variational approach we are also able to improve the calculation times and convergence behavior. Furthermore, the enhancement with plasticity and isotropic hardening allows to investigate the influences between damage and plastic strains to each other as well as the resulting influences to the cracks.

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S 4: Structural mechanics

Organizers: Sven Klinkel (RWTH-Aachen University)
Jens Wackerfuß (University of Kassel)

S 4 : Structural mechanics

Tuesday 14:00 - 16:00 Marienstr. 13, Ground floor, Lecture hall C

An algorithmic stress formula for energy conserving time integration in a mixed framework for polyconvex large strain elasticity

A. Janz (Karlsruher Institut für Technologie), P. Betsch (Karlsruher Institut für Technologie), C. Hesch (Universität Siegen) 14:00

The present work deals with a mixed variational formulation of elastodynamics along with an energy-momentum consistent discretization in space and time. The underlying continuum formulation relies on a polyconvex stored energy function [1]. In addition to the displacement field, further kinematic fields entering the polyconvex stored energy function are introduced by a newly proposed cascaded system of kinematic constraints. The corresponding mixed variational formulation is obtained by enforcing the kinematic constraints through a Hu-Washizu type variational functional. The newly proposed variational framework facilitates the design of new energy-momentum consistent discretizations in time. In addition to that, the mixed variational framework makes possible a wide variety of finite element discretizations in space. In the special case of a purely displacement-based discretization we obtain a new form of the algorithmic stress formula which is a typical feature of energy-momentum methods [2]. In particular, the new stress formula assumes a remarkably simple form when compared to previously proposed alternative stress formulas.

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A dual Craig-Bampton state-space approach for the approximation of damped systems

F. Gruber (Technical University of Munich), D. Rixen (Chair of Applied Mechanics, Technical University of Munich) 14:20

Dynamic substructuring techniques are very efficient to reduce the size of large models. Thereby the large model is divided into substructures, each substructure is analysed and reduced separately and then assembled into a reduced model of low order which approximates the behaviour of the original large model. During the assembly of the substructures some interface compatibility conditions are enforced between adjacent substructures. The most popular approach is a fixed interface method, the Craig-Bampton method, which is based on fixed interface vibration modes and interface constraint modes and assembles the substructures using interface displacements (primal assembly). Many other methods (MacNeal, Rubin, Craig-Chang) employ free interface modes, (residual) attachment modes and rigid body modes but also assemble the substructures in a primal fashion. On the other hand, the dual Craig-Bampton method employs free interface vibration modes, (residual) attachment modes and rigid body modes to build the reduction bases of the substructures, too, but assembles the substructures using interface forces (dual assembly). Commonly for the reduction of the substructures, all of these methods take only the mass and stiffness properties of the substructures into account and damping effects are neglected entirely. In this contribution the original dual Craig-Bampton method for the reduction and successive coupling of undamped systems will be modified for the case of general viscous damping. The final reduction is now based on the use of complex free-free dynamic vibration modes, (residual) flexibility modes and state-space rigid body modes. For the coupling of the substructures in state-space representation, a dual coupling procedure based on the interface forces between adjacent substructures is used. Thereby special attention has to be directed to the influence of the (residual) attachment modes since these modes can be computed for the displacement part and the velocity part of boundary degrees of freedom in the state-space vector. Moreover the rigid body mode concept has to be modified for the state-space with the possibility of generalized eigenvectors corresponding to multiple zero eigenvalues since not only regular eigenvectors corresponding to zero eigenvalues occur. An example is presented to show the potential of this dual Craig-Bampton approach for the case of general viscous damping and the computation of the aforementioned modes is demonstrated.

Application of Multipreconditioned Iterative Algorithms in Dual Domain Decomposition Methods for Structural Dynamics

M. Leistner (Technische Universität München), D. Rixen (Technische Universität München) 14:40

Although the idea of a multipreconditioned conjugate gradient method is already well known for many years, its application to domain decomposition algorithms [1] with parallel computing in mind is one of the latest and most promising developments in that field and subject of recent publications. The key property of the domain decomposition algorithms used here is the additive nature of their typical preconditioners which means that they work by summing up contributions from the individual domains. In the multipreconditioned case, these contributions are regarded as separate directions and are used to minimize the error in the space they span. In [2] this has been improved further by introducing criteria to select which directions will be considered separately. We review the

thus created state of the art multipreconditioned algorithms and asses their performance when applied in dual domain decomposition methods to solve problems in structural dynamics. Special emphasis is placed on the influence and consequential choice of the tuning parameter of the selection criterion. To thoroughly verify the behavior of the methods, different types of heterogeneous structures are considered.

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A polyconvex phase-field approach to fracture with application to finite-deformation contact problems

M. Franke (Karlsruhe Institute of Technology), M. Dittmann (Chair of Computational Mechanics, University of Siegen), C. Hesch (Chair of Computational Mechanics, University of Siegen), P. Betsch (Karlsruhe Institute of Technology) 15:00

Variationally consistent phase-field methods are able to efficiently simulate complex three-dimensional fracture problems (see [1, 2]). However, the developments for large deformations often exhibit a lack of numerical stability for different loading scenarios. In this talk we present a novel formulation for finite strain polyconvex elasticity by introducing a new anisotropic split based on the principal invariants of the right Cauchy-Green strain tensor which ensures polyconvexity of the resulting strain energy function (see [4]). Furthermore the variationally consistent Mortar contact algorithm is applied (see [3]) to handle complex contact boundaries. In order to improve accuracy a fourth order Cahn-Hilliard crack density functional is used. To account for the C^1 requirement the system is embedded in a sophisticated isogeometric framework with local refinement. The new polyconvex phase-field fracture formulation guarantees numerical stability for arbitrary hyperelastic materials. The performance of the proposed methods will be examined in representative numerical examples.

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Numerical Simulation of Contact by Optimal Transportation Meshfree (OTM) Method

D. Huang (Leibniz Universität Hannover), C. Weißenfels (Leibniz Universität Hannover), P. Wriggers (Leibniz Universität Hannover) 15:20

The Optimal Transportation Meshfree (OTM) method is a recently developed Galerkin type meshfree approximation scheme, hence it can be used for simulating both solid and fluid flows in a Lagrangian framework. This method can be viewed as an evolution of the finite element method (FEM) towards a meshfree simulation scheme. Due to the solely subdivision into nodes and material points in the OTM method, there is no body boundary surface existed for contact simulation. In this work, the impact-contact method, used in the material point method in order to compute contact case, is modified to the OTM method. Additionally, a new strategy is developed within the OTM framework which enforces the contact contribution directly by applying the penalty regularization. The contact is detected by the distance based support domain search algorithm, which means if one node from one body comes into the support domain of material point from another body, contact happens on this node. The impact-contact method is the most common approach in material point scheme to simulate contact, where the contact problem is seen as the impact of nodes from two bodies in the contact interface. The contact force is calculated by the difference between the nodal velocity before impact and the nodal velocity after impact. The penalty method is widely used in contact simulation by finite element method, where the slave node is projected onto the master surface and the contact force is calculated based on the penetration amount and penalty parameter. In case of the OTM in current work, the penetration is determined by projection of the slave node onto a virtual master surface due to the lack of continuous master surface. The contact algorithms are compared and validated by the benchmark simulation tests.

An explicit reduced order integration scheme for contact problems in structural dynamics

J. Shi (Institut für Allgemeine Mechanik), F. Bamer (RWTH Aachen University), B. Markert (RWTH Aachen University) 15:40

The numerical treatment of contact problems for dynamical systems is computationally demanding. The application of explicit time integration schemes forces the integration time step to be considerably small, therefore, a huge number of compuation loops has to be processed to evaluate the whole response function in the time domain. Especially, the detection of the contacting element surfaces demands expensive algorithms and must be performed in each computation step [1].

We present a model order reduction strategy that has been applied in materially nonlinear dynamical systems [2-3] and adapt this new strategy to a dynamical vibroimpact system. An aproiri response identification on the full system detects the nonlinear deformation patterns. Then, the reduced order computation is performed in a fractional amount of time in comparison to the full solution procedure.

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S 4 : Structural mechanics

Tuesday 16:30 - 18:30 Marienstr. 13, Ground floor, Lecture hall C

A note on the construction of vector-valued interpolation functions of Raviart-Thomas type

K. Steeger, F. Bertrand, J. Schröder (Institute of Mechanics, University of Duisburg-Essen), G. Starke, A. Schwarz 16:30

In the field of (mixed) finite element methods flux quantities can be used as an (additional) unknown field. The appropriate space for the approximation of flux fields is given by the Sobolev space $W^q(\mathrm{div}, \mathcal{B})$, given by $W^q(\mathrm{div}, \mathcal{B}) = \{\boldsymbol{P} \in L^q(\mathcal{B})^d : \mathrm{div}\ \boldsymbol{P} \in L^q(\mathcal{B})^d\}$, as only their divergence needs to be integrable in some sense. Since flux quantities are physically normal continuous and the chosen space implies this property across the edges of a triangulation, it is a suitable choice. Vector-valued Raviart-Thomas functions, see e.g. [1], can be used for the conforming discretization of $W^q(\mathrm{div}, \mathcal{B})$. In the engineering community, the application of such function is not widely spread. The reason therefore can maybe be found in the more or less complicated construction of the vector-valued ansatz functions, see e.g. [2]. Furthermore, almost no commercial finite element code is providing this type of interpolation. Thus, we want to consider two different ways of construction of Raviart-Thomas functions and discuss the resulting advantages and disadvantages. The first way is based on the evaluation of some outer and inner moments, whereas the second way uses the properties of the function at some nodal interpolation sites. The derivation will be restricted on the two-dimensional case and is shown detailed for a unit triangular domain. In order to preserve the $W^q(\mathrm{div}, \mathcal{B})$ conformity, we have to apply the Piola transformation on the basis functions previously defined on the unit triangle. The necessity of $W^q(\mathrm{div}, \mathcal{B})$ conforming interpolation functions will be discussed in detail. The interpolation will be tested using a least-squares mixed finite

element for solid mechanics with the displacements and the stresses as unknown fields, see e.g. [3].

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[2] Ervin, V., [2012], "Computational bases for RT_k and BDM_k on triangles", Comp. and Math. with Appl., Vol 64, pp. 2765-2774

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Remarks on a mixed least-squares finite element formulation for finite elasto-plasticity

M. Igelbüscher (University of Duisburg-Essen), A. Schwarz (University of Duisburg-Essen), K. Steeger (University of Duisburg-Essen), J. Schröder (University of Duisburg-Essen) 16:50

In the framework of elasto-plasticity the accurate approximation of the stress field is indispensable since it is mainly responsible for the evolution of plastic material behavior. In this contribution a mixed least-squares finite element formulation for geometrically nonlinear elasto-plasticity is discussed, where the stresses besides the displacements are used as an unknown field. The mixed least-squares finite element method (LSFEM) provides some numerical advantages e.g. a posteriori error estimator and the flexibility in the construction of suited functionals which are directly approximating the unknown field variables. Additionally, the provided LSFEM yields a minimization problem which is not restricted to the LBB or so-called inf-sup condition. This yields the possibility to choose the interpolation order and combinations without any constraints. The construction of the least-squares functional is based on the L^2-norm minimization of the residuals of a first-order system of differential equations, see e.g. [1]. Here, the residuals are given by the balance of momentum and a constitutive equation. The resulting functional is given as a two-field formulation depending on stresses and displacements. A drawback within the consideration of elasto-plasticity using the LSFEM is that the standard variational approach could lead to a discontinuity within the first variation of the functional initiated by the additional plastic constraint in the constitutive equation, see e.g. [3]. Thus, to avoid this drawback a modification of the method is performed to obtain a continuous first variation. Furthermore, a formulation is constructed by adding an additional redundant third residuum.
The underlying hyperelastic material law is given by a Neo-Hooke material model. Additionally, the plastic material response is described for simplicity by a isotropic von Mises yield criterion with linear hardening. Furthermore, the fulfillment of thermodynamic consistency and the occurring constraints in plasticity are investigated, see also [4]. For the integration of the flow rule depending on the plastic right Cauchy-Green deformation tensor an implicit exponential time integration scheme introduced first by

[5] is applied. The hardening law as well as the Karush-Kuhn-Tucker conditions are solved in the same way as in the small deformation theory, see e.g. [3]. For the numerical analysis we consider a three dimensional element of the type RT_mP_k, where m denotes the polynomial order of the stress approximation and the interpolation order of the displacements are given by the index k. In order to validate and compare the element performance a standard Galerkin element formulation is considered. The implementation and validation is performed using the AceGen and AceFEM packages, see [2].

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Subspace-based reduced-order modeling methods for inelastic structures

S. Tegtmeyer (Leibniz Universität Hannover), U. Nackenhorst (Leibniz Universität Hannover) 17:10

In order to save computational time and resources reduced-order modeling methods have been developed. Instead of solving the full system of equations resulting from a detailed Finite Element approximation of a complex model, the number of degrees of freedom is reduced to a smaller set of unknowns.

Subspace-based methods are one kind of reduced-order modeling methods. One advantage of these methods compared to a reduction method, where the behaviour of the system is entirely approximated by a new set of easy to solve equations, is that the structure of the system of equations is kept and therefore the same solving routines can be applied to the reduced model. The original system of equations is simply projected onto a subspace using a suitable projection matrix. These projection matrices may be depending on the loading of the model, e.g. Proper Orthogonal Decomposition, but most of them are mainly depending on the material and structure of the model, e.g. modal subspace, Krylov subspace, etc.

In this contribution, we study the effect and usability of subspace-based projection method for Finite Element models considering non-linear material behaviour. In this

case, iterative computations are necessary to determine the correct structural response. The tangential stiffness matrix depends on the deformation and changes for each iteration step. Once the stiffness matrix is rebuild, the system of equation needs to be resolved. These repeating computations can be performed more efficiently by reducing the system of equations. On the other hand, if the stiffness matrix changes, the perfectly fitted projection matrix will change. If we still use the same projection matrix as in the initial step, the reduced-order model becomes less accurate. If we update the projection matrix for each computation, the benefit of using a reduced-order model vanishes. The aim of this contribution, is the optimal ratio of updating and not updating the projection matrix for the model order-reduction technique of Finite Element models with non-linear material behaviour with respect to computational time and effort and accuracy of results.

Piecewise approach for matrix-interpolation-based parametric Model Order Reduction

M. Buchschmid (Technische Universität München), R. Rodríguez Sánchez (Technische Universität München), G. Müller (Technische Universität München) 17:30

In the design process of mechanical systems dynamic analysis is carried out in time domain or in frequency domain which implies solving the equation of motion several times. Usually the systems depend on a set of parameters which influence their responses. Thus the design process includes numerical simulations using a full-scale finite element model for each set of parameters which is computational demanding and time consuming, e.g. in the scope of frequency response. One approach to tackle this problem is by using parametric model order reduction (pMOR) methods. In this contribution a piecewise approach is presented for those pMOR methods based on interpolation in matrix manifolds and reduced order model (ROM) databases. The piecewise approach decreases the computational time and the stored data during the parametric-based simulation. A numerical example illustrates the suitability of this method in special for large frequency bands. The respective results using the piecewise pMOR approach is compared with the solution obtained using the corresponding full-scale model.

Co-rotational extension of the Logarithmic finite element method

C. Schröppel (University of Kassel), J. Wackerfuß (University of Kassel) 17:50

In the Logarithmic finite element (LogFE) method, a novel finite element approach proposed by the authors [1, 2], shape functions are defined on the Lie algebra of the deformation function. The deformation map is given by

$$\mathbf{x}^e(\boldsymbol{\xi}) = \overbrace{\exp\left(\sum_{i=0}^{n} u_i N_i(\boldsymbol{\xi})\, \mathfrak{e}_i\right)}^{\boldsymbol{\psi}^e(\boldsymbol{\xi})} (\mathbf{x}_0^e(\boldsymbol{\xi}))\,,$$

where $\mathbf{x}^e$ and $\mathbf{x}_0^e$ are the current and initial configurations of a finite element, n is the number of shape functions N_i present in the finite element, u_i are the degrees of freedom,

$\boldsymbol{\xi}$ is the parametrization of the finite element, and $\mathfrak{e}_i$ are vectors in the space of the Lie algebra. (In the standard Ritz-Galerkin approach, $\mathfrak{e}_i$ are simply basis vectors of the physical space.) $\boldsymbol{\psi}^e(\boldsymbol{\xi})$ is the deformation function applied to the finite element.
Given suitable shape functions, both translational and geometrically exact rotational field values at the nodes are linear functions of the respective degrees of freedom of the finite element system.
The initial discretized deformation space of the LogFE method is able to provide a good approximation of the exact solution for moderate deformations. However, for large deformations, a co-rotational update of the local coordinate systems, and thus, of the local discretized deformation spaces, is necessary to obtain good results.
To ensure convergence, a co-rotational variant of the LogFE method must meet the criteria of compatibility and of completeness. Compatibility means the preservation of continuity conditions at the boundaries of finite elements. Completeness means that under mesh refinement, the discretized solution converges to the exact solution, i.e. the discretized deformation space is dense within the exact solution space, which is generally assumed to be a Sobolev space of finite order.
Due to the presence of rigid body motion straining in LogFE formulations, the evaluation of the completeness criterion is of particular importance. Passing the *patch test*, applied to finite elements of finite size, guarantees the absence of rigid body motion straining of the discretized model. However, neither passing the finite-size patch test nor the absence of rigid body motion straining is necessary to pass the infinitesimal-size patch test [4, p. 257–8], which implies satisfying the completeness criterion given above.
The presentation includes an outline of the LogFE method and a discussion of co-rotational extensions of the LogFE method for beam elements with both Timoshenko and Bernoulli kinematics.

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An efficient Monte Carlo simulation strategy based on model order reduction and artificial neural networks

F. Bamer (RWTH Aachen University), A. Koeppe (RWTH Aachen University), B. Markert (RWTH Aachen University) 18:10

The computation of the nonlinear structural response to a dynamic excitation is generally time consuming as numerical schemes must be applied. Hence, the evaluation of the whole nonlinear response statistics to a set of random excitations can lead to an unrealizable task. In order to deal with this issue, a model order reduction (MOR) strategy [1,2] adapted to Monte Carlo (MC) simulations based on the proper orthogonal decomposition (POD) method is developed [3]. However, in order to produce a certain level of confidence, a considerably high number of samples must be computed. Consequently, the calculation time is high, although the adapted MOR is applied.
We introduce an extension to the existing MOR approach by the application of an artificial neural network (ANN). Hereby, within the POD reduced MC method, the ANN is trained in order to replace the whole reduced numerical integration procedure for one arbitrary excitation set. The ANN is trained as long as the approximation error is negligible compared to the POD reduced sample run. It is shown that by application of this new strategy a reasonable estimation of the distribution function can even be produced in the tail region within a feasible computation time period.

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S 4 : Structural mechanics

Wednesday 14:00 - 16:00 Marienstr. 13, Ground floor, Lecture hall C

Path Following Algorithm in Static Nonlinear Structural Analysis: State of the Art and Simple New Method Implementation

W. Guggenberger (Graz University of Technology) 14:00

In the framework of advanced static geometrically nonlinear structural analysis, i.e. neglecting any viscous and inertia effects by mechanical modeling considerations, the path following algorithm plays an important role. Since, it is only with its distinct help that efficient and robust practical analyses may be performed. From the perspective of a long - term scientific analyst a large amount of practical path following - experience may ac-

cumulate including encounters with uncomfortable path following situations. This may lead to strong desire for improvement or even modification of existing path following strategies but also to developing concrete ideas about the realisation of such possible improvements. Examples of such improvements are 1. optional analysis control by a single fixed but otherwise freely selectable system parameter, 2. optional automatic change of the controlling system parameter, 3. simple, robust and transparent procedure for analysis reversal or analysis continuation (multiple times if needed or desired). Further improvements are 4. automatic calculation of specific deformation states which are designated by fixed values of individual specific system parameters, i.e. deformation components, load factor etc, 5. automatic recognition of states of system parameter reversals and optional search for them, 6. simple and transparently usable scaling rules or weighting rules for the different types of mechanical system parameters by introducing type - specific reference quantities etc. For better understanding, the distinct states of system parameter reversals are designated by the fact that any single system parameter, eg the load parameter, traverses an extremal point and as such reverses its „sign“ or its „direction“ of increase.
In this paper the essential theoretical and practical aspects of a path following algorithm as well as its essential working purpose and its essential working mode of operation are worked out and presented in simple understandable terms. Based on this background knowledge the various common forms of path following algorithms are constructed and compared, leading to stepping - forward algorithms which differ in the (internal) algorithmic mode of operation as well as in the accompanying (external) user possibilities of algorithmic control.
Finally the simplest possibility of a path following algorithm is chosen and implemented which at the same time turns out most primitively structured on the one hand but most versatile in its practical usability on the other hand. The efficiency of this novel proposed path following methodology is demonstrated by worked benchmark examples and by real world examples.

Non-unique Equilibria of a Statically Indeterminate System with Coulomb Friction

W. Steiner (University of Applied Sciences Upper Austria) 14:20

The goal of this contribution is to show that the Coulomb friction model in a statically indeterminate system can result in ambiguous states of equilibrium. We demonstrate that a simple framework under specific external loading is in equilibrium and satisfies all conditions of Coulomb friction in the support points for several states of stress and deformation. The presented problem is motivated by the example of a two dimensional elastic body discussed in [1] where non-unique static solutions were found, too. In our presentation, a new method [2] which extends Castigliano's theorem to problems with Coulomb friction is applied to efficiently analyze numerous states of sticking and sliding of the framework's supports.

[1] P. Hild, An example of nonuniqueness for the continuous static unilateral contact

model with Coulomb friction, C. R. Acad. Sci. Paris, Ser. I 337 (2003).

[2] W. Steiner, The use of Castigliano's theorem in Coulomb friction problems, Acta Mechanica, September 2014, Volume 225, Issue 9, pp 2471-2483.

An objective and locking-free finite-element formulation for geometrically exact Kirchhoff rods

M. Schulz (TU Braunschweig / Institut für Festkörpermechanik), M. Böl (TU Braunschweig) 14:40

Slender mechanical objects, e.g. beams, are prevalent in problems of mechanical, aerospace, and civil engineering. These objects distinguish themselves by a predominant dimension in length direction which is much larger than the dimensions perpendicular to it. This circumstance allows for the derivation of one-dimensional mechanical theories which provide access to analytical solutions on the one hand and lay the foundation for numerically efficient finite-element beam formulations on the other hand.
For very slender beams it can be appropriate to assume vanishing shear-deformations which means that the cross-sections remain undeformed. This kinematic constraint is also called "Kirchhoff constraint" based on his work from 1859 where he presented the first formulation capable of describing large three-dimensional deformations of such a beam. Despite this long tradition there is only one objective, locking-free finite-element formulation for curved Kirchhoff beams which is based on constraining the rotation variation to satisfy the Kirchhoff constraint. This approach results in the need for C^1-continuous shape functions and an elaborate definition of an objective reference frame.
In contrast, here a new Kirchhoff beam finite-element formulation will be presented by constraining the variation of the displacement of the center-line which goes through the centroids of all cross-sections. This strategy has the advantage that it requires only C^0-continuous shape functions and no definition of a reference frame. The objectivity, path-independence, absence of locking phenomena, and accuracy of this new formulation are investigated and confirmed using appropriate numerical examples.

Bending of viscoplastic cables

V. Dörlich (Fraunhofer Institut für Techno- und Wirtschaftsmathematik), J. Linn (Fraunhofer Institut für Techno- und Wirtschaftsmathematik), S. Diebels (Universität des Saarlandes) 15:00

Cables are flexible objects with a high aspect ratio and can be described in terms of the sectional forces and moments. Therefore, a model based on the physically correct Cosserat rod theory is used in this work. It uses geometrically exact kinematics relating configuration variables and objective strain measures, balance equations in terms of the sectional quantities and constitutive equations for the sectional forces and moments formulated in the deformation measures [1].
Since cables consist of several layers [2], internal dissipation effects like friction, geometrical hindrance and delamination influence their deformation behavior. Moreover, cables typically contain different kinds of materials, e.g. polymers or metals. Consequently,

the material behavior varies from elastic to viscoplastic, depending on the constituents. This work focuses on the investigation of the behavior of cables during bending, which is a deformation mode relevant for plastic behavior. Up until now, it is state of the art to use three-point bending tests to determine the bending stiffness of cables [3]. This kind of experimental setup yields a deformation state where the bending moment increases linearly from the ends of the specimen to the middle, i.e. the curvature is not constant along the cable axis. Additionally, normal and shear forces occur in real bearing situations and influence the kinematics of the specimen in contrast to theory. Therefore, a new experimental setup was designed in order to perform pure bending experiments on cables. It enables the measurement of the bending moment without any influence of normal or shear forces. The constitutive equation for bending, i.e. the bending moment as function of bending curvature, and its parameters can hence be accessed directly in the pure bending experiment.
This contribution will present the pure bending device and give a comparison of both bending experiments on viscoplastic cables.

[1] J.C. Simo. A finite strain beam formulation: the three dimensional dynamic problem - Part I. Comp. Method. Appl. M. 49 (1985), 55–70.

[2] V. Dörlich, J. Linn, T. Scheffer, S. Diebels. Towards Viscoplastic Constitutive Models for Cosserat Rods, Arch. Mech. Eng. 63 (2016), 215–230.

[3] V. Dörlich, S. Diebels, J. Linn. Investigation of elastoplastic effects of cables under large spatial deformation, Proc. Appl. Math. Mech. 15 (2015), 185–186.

Geometry model for twisted cords and its application to FE analyses of textile reinforced rubber components

N. Heinrich (Chemnitz University of Technology), H. Donner (Chemnitz University of Technology), J. Ihlemann (Chemnitz University of Technology) 15:20

Many rubber components contain textile reinforcement as an essential feature to provide certain functionality. This contribution focuses on air springs commonly used in commercial vehicle suspension systems. Air spring bellows for these applications are usually equipped with two plies of reinforcing cords. The cords are manufactured by twisting yarns, which, in turn, are obtained from twisting filaments. As a result, cords exhibit not only a very complex geometry but also strong anisotropic material behavior.
In FE analyses, these properties are often neglected by assuming a one-dimensional stiffness [1]. However, in order to capture local stress and strain distribution in cord-rubber composites both geometry and anisotropy must be taken into account. For that purpose, a geometry model for representing twisted cords in space and suitable material assignment techniques are suggested in this contribution.
The cord geometry model is built in two steps. First of all, the twisting process is simulated to identify the free parameters of an analytical model describing the cross

section [2]. Then, this cross section is translated along a space curve and rotated about it according to the cord's twist. In the context of FE modelling, this geometry model could be employed by creating separate parts for each yarn and the rubber matrix. However, as this would lead to an irregular mesh with a high amount of elements, the composite is modelled as a whole instead. Afterwards, the geometry model is used to identify the material region that any integration point belongs to [3]. In case of an integration point lying inside one of the yarns, a transversely isotropic material model with the filament's path as preferred direction is assigned. Otherwise, the integration point must belong to the rubber matrix and receives a hyperelastic material model. With this approach, FE models for air springs resolving the inner structure of the bellows in great detail can be created. Moreover, a validation of analysis results with experimental data shows good agreement.

[1] S. Oman and M. Nagode, On the influence of cord angle on air-spring fatigue life, Engineering Failure Analysis 27 (2013), 61-73

[2] H. Donner and J. Ihlemann, On the efficient finite element modelling of cord-rubber composites, Constitutive Models for Rubber VIII (2013), 149-155

[3] J. Kreikemeier, Modelling of Phase Boundaries via the GAUSS-Point Method. Technische Mechanik 32 (2012), 658-666

Projection and variational approaches to spectral analysis of thick elastic beams

G. Kostin (Institute for Problems in Mechanics RAS) 15:40

A projection approach to modelling of natural vibrations for 3D elastic beams is proposed based on polynomial semi-discretization of displacement and stress fields. This projection technique is developed as modification of the Petrov–Galerkin method in the frame of the method of integro-differential relations (MIDR) [1], in which the local constitutive laws are replaced by an integral equation. As a result, the original eigenvalue problem in partial differential equations is approximated by a system of ordinary differential equations (ODEs). The approximations include a polynomial expansion of finite dimension over two coordinate components and unknown functions over one remaining component [2].

As compared with the classical Bubnov–Galerkin method rely on a variational formulation, the projection approach possesses some advantages: it provides explicit error estimates and supposes the exact implementation of the initial, boundary, and momentum balance conditions. Some drawbacks of the variational method are in doubling the dimension of the resulting ODE system in accordance with the Euler–Lagrange conditions.

The variational statement of the eigenvalue problem in the linear theory of elasticity is: Find the displacement vector $w(x) \in \mathbb{R}^3$, the momentum density $p(x) \in \mathbb{R}^3$, and the symmetric stress tensor $\sigma(x) \in \mathbb{R}^{3\times 3}$ in a spatial domain $x = (x_1, x_2, x_2) \in \Omega \subset \mathbb{R}^3$ that

are a stationary point of the functional $\Phi_-[w,p,\sigma]$, i. e. $\delta\Phi_- = 0$, where

$$\Phi_\pm = \int_\Omega \varphi_\pm \mathrm{d}\Omega, \quad \varphi_\pm = \frac{1}{2}(\rho v\cdot v \pm \xi : C : \xi), \quad v := w_t - \frac{p}{\rho}, \quad \xi := \frac{1}{2}(\nabla w + \nabla w^\top) - C^{-1} : \sigma,$$

subject to Newton's second law $p_t = \nabla\cdot\sigma$ and homogeneous boundary conditions

$$w = 0 \quad \text{for} \quad x \in \Gamma_w \quad \text{or} \quad \sigma\cdot n = 0 \quad \text{for} \quad x \in \Gamma_\sigma \quad \text{with} \quad \bar\Gamma_w \cup \bar\Gamma_\sigma = \Gamma = \partial\Omega \quad \text{and} \quad \Gamma_w \cap \Gamma_\sigma = \emptyset.$$

Here, $\rho(x)$ denotes the volume density, $C(x)$ is the elastic modulus tensor, $n(x)$ is the outward normal to the boundary Γ.
The projection formulation of the problem is as follows:
Find the displacement, momentum, and stress fields obey the integral relation

$$\int_\Omega \rho v\cdot u + \xi : \tau \mathrm{d}\Omega = 0 \quad \text{for} \quad \forall u \in L^2(\Omega,\mathbb{R}^3) \quad \text{and} \quad \forall \tau = \tau^\top \in L^2(\Omega,\mathbb{R}^{3\times 3})$$

subject to the above-mentioned constraints. The vector function $u(x)$ and the tensor function $\tau(x)$ define the test space for numerical solution according to the Petrov–Galerkin method. The values of the functional $\Phi_+[w,p,\sigma] \geq 0$ is used to estimate the resulting solution quality.
As an example of thick beams, a homogeneous isotropic elastic body occupying the domain $\Omega = \{x \in \mathbb{R}^3 : |x_i| < a_i,\ i = 1,2,3\}$ – right prism with a quadratic cross section – is under study. The lateral faces of the prism are free of external loads, whereas the displacements are fixed and equal to zero on its bases. Due to the problem symmetry, natural vibrations of the prismatic beam are decomposed into six independent groups of eigenmodes, namely, two types of "breathing" motions, two types of lateral vibrations, torsions, and longitudinal vibrations. Spectrum characteristics of the beam and their specific properties caused by the domain symmetry and beam thickness are discussed.

[1] Kostin G., Saurin V. Integrodifferential Relations in Linear Elasticity. De Gruyter, Berlin, 2012.

[2] Kostin G., Saurin V. Modelling and analysis of the natural vibrations of a prismatic elastic beam based on a projection approach. J. Appl. Math. Mech. 75(6) 700–710 (2011).

S 4 : Structural mechanics

Wednesday 16:30 - 18:30 Marienstr. 13, Ground floor, Lecture hall C

Accounting for transverse shear in shell-based ply-level models of layered composites

M. Todt (TU Wien, Institute of Lightweight Design and Structural Biomechanics), M. Schwab (TU Wien, Institute of Lightweight Design and Structural Biomechanics), F. Rammerstorfer (TU Wien, Institute of Lightweight Design and Structural Biomechanics), H. Pettermann (TU Wien, Institute of Lightweight Design and Structural Biomechanics) 16:30

Shell-based ply-level (SPL) models are a computationally efficient approach to separately treat intra-ply damage and delamination in finite element simulations of layered composite structures.

Within conventional SPL models the individual plies are modeled using shell elements and the interfaces between adjacent plies are represented by infinitely thin and quasi-rigid cohesive zone elements (CZE) possessing a traction-separation behavior. As a consequence of this modeling strategy the out-of-plane stresses are not captured correctly and the predicted elastic response of the structures is way too stiff with respect to transverse shear loading.

In this talk, an extended SPL approach is presented allowing to overcome the issues of conventional SPL models by assigning the CZEs as subset of the 3D continuum behavior. This subset comprises the out-of-plane properties of the adjacent plies and the properties of the interfaces between the plies.

The applicability of this approach is verified for the example of an isotropic beam as well as for thick layered composite plates with different lay-ups subjected to transverse shear loading. Corresponding models with continuum element discretization are used as reference. The proposed extended SPL approach resembles the continuum model solutions in terms of transverse shear stresses and deformations almost perfectly without compromising the membrane stresses in the shells. The differences between the results of the extended SPL models and the continuum models are in general lower than 1%. Slightly larger differences in the deformations only occur for composite lay-ups which show a strong bending-to-twisting coupling.

Concluding it can be said, that for the modeling of layered composite structures the extended SPL approach provides a high reliability of the results in combination with high computational efficiency.

An Isogeometric Inverse Method for Finding Unknown Surface Tractions on Shells

B. Vu (Bauhaus-Universität Weimar), X. Duong (RWTH Aachen University), T. Lahmer (Bauhaus-Universität Weimar), H. Park (Boston University), T. Rabczuk (Bauhaus-Universität Weimar) 16:50

This article presents an inverse approach used to recover the applied loads and displacements on thin shell structures formulated by nonlinear kinematics and nonlinear constitutive models. The inverse formulation is tackled by gradient based optimization algorithms of computed and measured displacements at a number of discrete locations. Various numerical simulations are performed to capture either the non-instability shape changes or the shape changes that occur due to instabilities (i.e. snapping and buckling) of shell structures. Some representative examples will be presented and validated. The results obtained show a good performance and applicability of the proposed algorithms to manufacturing applications of high-fidelity shell structures.

A layered shell element for the computation of interlaminar and thickness normal stresses

G. Knust (Technische Universität Darmstadt, Fachgebiet Festkörpermechanik), F. Gruttmann 17:10

The prediction of interlaminar stresses is essential for the design of composite structures. In this work a layered shell element for the computation of laminated structures is proposed. The shell kinematic is based on the Reissner-Mindlin theory with an inextensible director field.
Further a multi-field functional is introduced including the global shell equations and additional Euler-Lagrange equations. These Euler-Lagrange equations enforce the correct shape of warping through the thickness and lead to continuous transverse shear stresses at layer boundaries [1].
This leads to a mixed hybrid shell element, after elimination of stresses, warping and Lagrange parameters on element level. The resulting shell element has the usual 5 or 6 degrees of freedom per node, making it possible to apply this element to complex geometrical structures.
An extension of the element to compute stresses in thickness direction is shown, in order to estimate and predict interlaminar failure. The computed results show good agreement with 3D solid shell models. Various examples for the computation of interlaminar shear stresses and thickness normal stresses are shown and compared to results of 3D elements.

[1] F. Gruttmann, W. Wagner, G. Knust. A Coupled Global-Local Shell Model with Continuous Interlaminar Shear Stresses. Comp. Mech. 57 (2016) 237–255.

Separate control meshes for displacements and rotations for a shear locking free isogeometric Reissner-Mindlin plate

G. Kikis, S. Klinkel (RWTH Aachen University) 17:30

In the analysis of plate and shell bending problems using an isogeometric Reissner-Mindlin approach, transversal shear locking effects may occur especially for thin structures. One possibility to overcome locking effects is to increase the polynomial order of the NURBS basis functions. However, there are certain examples where this method shows some deficiencies, like oscillations. For low polynomial degrees, there exist only a

few effective concepts for the elimination of locking effects. One is the enhanced assumed strain (EAS) method which is used in finite element formulations and which is sensitive to distorted element geometries. Beirão da Veiga et al. [1] introduced a new approach for a Reissner-Mindlin plate formulation where the displacements and rotations of the mesh are approximated using different control meshes. The physical space of the structure always remains the same. Hence, the method is in accordance to the isoparametric paradigm. However, the shape functions for the approximation of the displacements and the rotations may have different polynomial degrees and number of control points. In this way, the compatibility requirement for pure bending is fulfilled and shear locking is avoided. The method is tested for an isogeometric Reissner-Mindlin plate formulation, which is based on a degenerated shell formulation [2]. Basic examples are chosen and the results are compared to the unaltered isogeometric Reissner-Mindlin plate and the finite element method using MITC elements. The results show that the method has similar accuracy and efficiency as the MITC element and is also applicable for skew element geometries.

[1] L. Beirão da Veiga, A. Buffa, C. Lovadina, M. Martinelli, and G. Sangalli. An isogeometric method for the Reissner-Mindlin plate bending problem. Comput. Methods Appl. Mech. Engrg. 209-212 (2012) 45-53.

[2] W. Dornisch, R. Müller, S. Klinkel. An efficient and robust rotational formulation for isogeometric Reissner–Mindlin shell elements. Comput. Methods Appl. Mech. Engrg. 303 (2016) 1-34.

ASSESSMENT OF A MULTI-THREADED FEAP PERFORMANCE IN COMPOSITE SHELLS COMPUTATIONS

P. Jarzebski (Karlsruher Institut für Technologie), K. Wisniewski (Institute of Fundamental Technological Research Polish Academy of Sciences), W. Wagner (Karlsruher Institut für Technologie) 17:50

Multi-scale models used in computation of composite shells require a significant computational power and, therefore, a finite-element code should take advantage of such techniques as: 1) parallel solvers, e.g. PARDISO, MUMPS, PaStiX, (2) parallelization of a loop over elements using, e.g. OpenMP, and (3) domain decomposition and spreading tasks over a cluster of computers, using e.g. MPI. A significant programming effort is needed to convert a large and complicated existing FE code into a parallel one; in this paper, we focus on the first two techniques.

Personal computers have processors with several (2-32) cores, which make them shared memory architectures, for which communication is implicit. An appropriate parallelization technique for such architectures is a threading parallelism, which may be based on the OpenMP standard, specifying parallelization in terms of compiler directives, library routines and environment variables. OpenMP defines the 'fork-join' parallelism, because it launches multiple parallel threads (fork) in parallel regions of a code and joins them into a single thread (the master one) for serial processing in non-parallel regions.

We parallelize a loop over elements in the research code FEAP (Taylor, 2014) using OpenMP to enable parallel computations on a multi-core machine with shared memory. This requires several modifications of the code and a specific method of synchronization for assembling, see (Jarzebski, Wisniewski & Taylor, 2015). Besides, the interface to the parallel sparse solver HSL MA86 (Hogg & Scott 2010) is implemented, which enables the use of various re-ordering methods. The so-parallelized FEAP is designated 'ompFEAP' and preliminary tests show its very good performance (Jarzebski, Wisniewski, 2016).
In this presentation, we assess the performance of ompFEAP on the machine with up to 32 cores using several shell benchmarks. Computations are performed on the bwUniCluster of the Karlsruhe Institute of Technology, which built of nodes with either two Octa-core Intel Xeon E5-2670 processors or four Octa-core Intel Xeon E5-4640 processors. We show that the applied parallelization implies a significant speedup and reduces the time of computations at the expense of an only small increase in memory usage.

Hogg J., Scott J. (2010). An indefinite sparse direct solver for multicore machines. Technical Report TRRAL-2010−011.
Jarzebski P., Wisniewski K., Taylor R.L. (2015). On parallelization of the loop over elements in FEAP. Computational Mechanics 56(1), 77–86.
Jarzebski P., Wisniewski K. (2016). Performance of the parallel FEAP in calculations of effective material properties using RVE. Advances in Mechanics: Theoretical, Computational and Interdisciplinary Issues, CRC Press/Balkema, 241-244.
Taylor R.L. (2014). FEAP Ver. 8.4.

Topology Optimization for Injection Molding of Short Fiber-Reinforced Plastics

F. Ospald (TU Chemnitz), R. Herzog (TU Chemnitz) 18:10

Today there exists a huge demand for technologies which enable and facilitate the mass production of fiber reinforced composites. Injection molding of short fiber reinforced plastics (SFRP) is a quite popular method especially in the automotive industry, providing high stiffness levels on the one hand and complex moldable shapes on the other hand. Due to the high cost of mold production and injection molding machines, nowadays lots of research is done to improve models and to develop software for the simulation of this process. This allows to detect problems with the mold design and optimization of the part performance and quality at an early stage of the development.
In the case of SFRP injection molding, the mechanical properties of the finished part are mainly influenced by the local fiber orientation, which itself depends on the shape/topology of the part. We investigate an approximate approach for the compliance-based topology optimization for such parts, by replacing the costly filling and fiber orientation simulation by the solution of an eikonal equation which determines the principal fiber orientation. The problem is formulated as a variational problem and discretized with the finite element method. The optimization problem is then solved using the classical SIMP method in combination with a transversely isotropic material law. As a second application we consider topology optimized parts for the identification of material parameters in the sense of optimal experimental designs.

S 4 : Structural mechanics

Thursday 14:00 - 16:00 Marienstr. 13, Ground floor, Lecture hall C

Experimental and numerical investigation of a walking soft robot

K. de Payrebrune (TU Freiberg) 14:00

In many industrial and biomedical fields, robots and automata are used to reduce dangerous or repeatable tasks people do not wish to perform, to overcome human limitations in strength and speed, or to operate in hostile environments where humans are unable to work [1, 2]. Recently a new kind of "bio-inspired" robots, so called soft robots, has been the object of extensive research. Thereby, the research is motivated by the potential benefits of soft robots in applications to healthcare, cooperative human assistance, service robots and biomechanically compatible interactions [2, 3, 5]. With the absence of a skeleton-like structure and the use of soft materials, complex locomotion or movements of the soft robot are possible and hence, situation-related adapted behavior feasible. However new control strategies and mathematical models are required to advance the field of soft robots and to take their special characteristics into account [5, 6].
This work presents a mathematical model based on the nonlinear rod theory of Euler to reproduce the locomotion of a pneumatically actuated rubber based continuous soft robot. Therefore, the complex geometry of the soft robot is reduced to a material curve in space for which the flexural rigidity is identified experimentally. Further, the pneumatic actuation is converted into a non-constant pressure dependent curvature, which is the driving input parameter in the model. Solving the balance of linear and angular momentum, the deformation of the soft robot can be predicted under consideration of applied forces and given boundary conditions.
To analyze the locomotion of a quadruped soft robot, its geometry is represented by a segmented rod model. The actuation of each robot segment can be controlled separately and an actuation sequence identified such that the robot moves forward. For the simplest controllable gait of a caterpillar, the locomotion is studied for different pressures. Although the rod theory simplifies the geometry of the robot strongly, very good agreements between measurements and simulations are found. This strengthens the idea to use the computational efficient but geometrically simple rod theory to model complex dynamically actions of soft robots.

[1] M. Hägele and K. Wegener. Service-Roboter-Visionen. Hanser Verlag, (2004).

[2] C. Majidi. Soft Robotics SoRo, 1, 5 –11 (2013).

[3] S. Kim, C. Laschi and B. Trimmer, Trends in Biotechnology, 31, 287 –294 (2013).

[4] R. Pfeifer, M. Lungarella, and F. Iida, Commun. ACM, ACM, 55, 76 –87 (2012).

[5] F. Iida and C. Laschi, Procedia Computer Science, 7, 99 –102 (2011).

Thermomechanical measurement of a brake disc

A. Lamjahdy (RWTH Aachen University), B. Markert (RWTH Aachen University) 14:20

The experimental study of the thermomechanical behaviour of disc brakes is reported. The goal of this study is to better understand and explain the thermomechanical effects of disc brakes by use of an advanced measurement system. Temperature measurements with an infrared camera, pyrometer and thermocouples have been carried out on the rubbing surface of brake discs and brake pads on a flywheel test bench. The mechanical behaviour is determined with a high-speed detecting capacitive sensor. Based on the advanced measurement system, a detailed description of the occurring phenomena is possible. From these experimental researches, a scenario of brake cycles is conducted. Moreover, the change of the pad stiffness and pad contact length is studied [1], [2]. Finally, a detailed discussion of the observed experimental behaviour and the theoretical approaches [3] is proposed.

[1] Dufrenoy, P., Weichert, D., *Experimental Analysis of Hot Spotting in Sliding Systems, Springer Science, vol. 1, pp. 1-12, 2013.*

[2] Wicker, P., *Influence des garnitures de frein sur les sollicitations thermiques des disques TGV et consequences sur les risques de fissuration, Ph.D. Thesis, Ecole Central de Lille, 2009.*

[3] Markert, B., *A survey of selected coupled multifield problems in computational mechanics, Journal of Coupled Systems and Multiscale Dynamics, vol. 1, issue 1, pp. 22 - 48, 2013.*

An experimental and numerical study of gas pressure forming under shock-wave loading

N. Shirafkan (RWTH-Aachen University), B. Markert (RWTH Aachen University) 14:40

Explosive forming is an unconventional technique, in which a fluid is used as the pressure transmission medium. In gas pressure forming process, such as explosive forming, a plate is plastically deformed by means of high kinetic energy. Good surface due to reduced friction, reducing the number of processes or tooling and higher formability of some materials in comparison to conventional methods are the principal advantages of this method. To optimize the forming process, the knowledge of material behavior under very high pressures and deformation rates is required.

This study aims to characterize the high strain rate phenomena for different metals by performing shock-wave tube tests and simulating those with ABAQUS. Series of shock-wave tests are performed for circular metal plate specimens to obtain the global displacement curves. The specimen deformation is controlled through selective material removal during sheet preparation using milling machines. For the numerical simulations, the Johnson-Cook model is used to predict the high strain rate phenomena during the tests. Some conclusions about the different material deformations will be presented.

[1] Sandeep P.Patil, Madhur Popli, Vahid Jenkouk, and Bernd Markert: *Numerical modelling of gas detonation process of sheet metal forming*, Journal of Physics: Con-

ference Series. Springer International Publishing,(2016).

[2] Yasar, M: *Gas detonation forming process and modeling for efficient spring-back prediction*, Journal of materials processing technology 150, 270 – 279 (2004).

[3] Syn, C., O'Brien, M., Lesuer, D. Sherby, O: *An Analysis of Gas Pressure Forming of Superplastic AL 5083 Alloy*, International Conference on Light Materials for Transportations Systems (2001).

A machine-learning approach to load-monitoring based on guided waves

D. Hesser (RWTH Aachen University), B. Markert (RWTH Aachen University) 15:00

The research field of structural health monitoring (SHM) describes the way to state the structural integrity. The research objectives are broadly diversified, which are all addressing the improvement of SHM technologies. The goal of this paper is to optimise the robustness over the complete lifetime. In this context, it is important to optimise the capability of sensor networks by applying intelligent signal processing models. These intelligent systems predict the health state based on acquired data in a real-time environment. Piezoelectric sensor networks and guided-wave based analyses are combined with machine learning to create an efficient load-monitoring routine. This load-monitoring approach is chosen to track any change in the environmental conditions, which causes most of the problems in a reference signal based damage approach. The operational conditions will change continuously over the complete lifetime. Therefore, the output of the load-monitoring method can be used to compensate the acquired signals and to optimise the robustness of SHM systems. In addition to that, the machine learning algorithm is capable to deal with a big database, to evaluate the data in real-time and to solve the inverse problem. The analysed system will consist of multiple piezoelectric elements to apply guided-waves through the structure and to measure the wave response. The wave response will change based on the health state or loading condition. Finally, the proposed method will expose the influence of loading conditions to improve the performance and robustness of future SHM systems by means of machine learning and smart elements.

[1] Hesser, D.F., Markert, B.:*Excitation strategies for vibration based damage detection using piezoelectric transducers and machine learning*, PAMM, 16: 141–142, 2016, doi:10.1002/pamm.201610059

[2] Hesser, D.F., Markert, B.:*Optimal Frequency selection for vibration based damage detection using pattern recognition*, 8th European Workshop on Structural Health Monitoring (EWSHM), Bilbao, Spain, July 2016.

Multi-stage parameter identification of structural models from experimental data of varying assembly levels

B. Greiner (Universität Stuttgart), J. Wagner (Universität Stuttgart) 15:20

Classical applications of the Finite Element Method (FEM) in the aerospace industry include structural models of a high variety. For instance, models are used to predict dynamical properties during all design and integration phases such as qualification and characterization tests as well as in regular operation. During development, test results can be used for the identification and updates of model parameters, which in turn can then be employed to improve the prediction of other, not yet tested or not testable items. In recent years, the development of structures with electromechanical components, such as actively controlled subsystems or systems with structural health monitoring, has extended the amount of available data suitable for parameter identification in operational conditions even beyond the development phase.
The contribution presents an approach of using measurement data from different stages of assembly levels for the identification and update of model parameters not only of individual part and assembly models but also for the integrated entire structure. The method is applied to a simple trusswork test structure as well as to the Stratospheric Observatory for Infrared Astronomy's (SOFIA) Telescope Assembly. Experimental modal analyses of subassemblies and the whole telescope assembly as well as vibration measurements during operational conditions are used to estimate model parameters for an updated finite element model derived from legacy models created during the observatory's design phase.
While estimating parameters for subassembly models is often more intuitive than a global approach, estimation uncertainties propagating onto higher assembly levels have to be considered when assessing the model accuracy of a composed complete model.

Thermally loaded elastic-plastic shrink fit with FGM-hub

T. Apatay (Gazi University), E. Arslan (Inonu University), W. Mack (TU Wien) 15:40

As shrink fits are a simple and cost-effective means of transfer of moment, they frequently are found in mechanical engineering. Some examples are shrunk-on rings, armature bandages, or tires of railway wheels [1]. Since under certain circumstances a partially plastic design for better utilization of the material is admissible [2], not only elastic but also elastic-plastic states have been studied comprehensively (see the application-oriented monograph [3]). In further investigations, special attention was paid on the one hand to the widely-used thermal assembly process (e.g. [5]) and on the other hand to the behaviour under operating conditions like heating and/or rotation (e.g. [5]). Since for given geometry of the shrink fit and friction coefficient at the interface between inclusion and hub the transferable moment depends solely on the interface pressure, the latter should be as large as possible; as mentioned above, this may be achieved by a partially plastic design, for example. Moreover, it becomes increasingly important in engineering practice to minimize the weight of the device while maintaining a good performance of the shrink fit.

Hence, an interesting option is the use of a functionally graded material (FGM), particularly for the hub [6]; as is well known, in a machine part of FGM the material properties like modulus of elasticity, density, coefficient of thermal expansion, and yield stress vary continuously and can - to a certain extent - be tailored in an appropriate way. Whereas in [6] a purely elastic shrink fit of this kind (under plane stress conditions, corresponding to a thin hub) was considered, the aim of the present study is to investigate the essential features of an elastic-plastic design, taking operation at elevated temperature into account. The material properties are presupposed to vary according to a power law in the radial direction; in particular, the case of radially decreasing density of the hub is considered. The latter property may be realized, e.g., by using a steel/aluminum FGM, which can be produced by a powder-metallurgical process. Specifically, the case of a shrink fit with solid inclusion under plane strain conditions subject to homogeneous heating is considered. It is shown that for a sufficiently large ratio of outer surface radius to interface radius a good performance of the device can be maintained while a substantial saving of weight as compared to a homogeneous hub is possible. All the results are derived by analytical means, and the effect of various degrees of grading is discussed. While numerical examples are given particularly for a hub of steel/aluminum FGM, the general results nevertheless are applicable to any FGM with similar ratios of the material properties of the constituents.

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[2] U. Gamer. A concise treatment of the shrink fit with elastic-plastic hub. Int. J. Solids Struct. 29 (1992), 2463-2469.

[3] F.G. Kollmann. Welle-Nabe-Verbindungen. Konstruktionsbücher Bd. 32. (Springer, Berlin, 1984).

[4] M. Lorenzo, J.C. Perez-Cerdan, C. Blanco. Influence of the thermal assembly process on the stress distributions in shrink fit joints. Key Eng. Mater. 572 (2014), 205-208.

[5] W. Mack, M. Plöchl. Transient heating of a rotating elastic-plastic shrink fit. Int. J. Eng. Sci. 38 (2000), 921-938.

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S 4 : Structural mechanics

Thursday 16:30 - 18:30 Marienstr. 13, Ground floor, Lecture hall C

Modelling of shell structures using the scaled boundary finite element method

M. Wallner, H. Gravenkamp (University of Duisburg-Essen), C. Birk (University of Duisburg-Essen) 16:30

In view of recent trends to lightweight structural designs, the numerical modelling of shell structures is a subject of high interest. Here, major challenges are associated with locking effects. The dominating locking effect for shells is membrane locking, a stiffening phenomenon where parasitic membrane stresses occur in pure bending situations.
Several approaches exist to avoid locking when modelling shell structures. These include reduced integration, assumed natural strain approaches, enhanced assumed strain methods, and discrete strain gap formulations, for example.
This contribution presents a first approach to the numerical analysis of shell structures using the scaled boundary finite element method (SBFEM). The SBFEM is a semi-analytical technique which combines the advantages of the finite element method and the boundary element method. As in the boundary element method, only the boundary of the domain is discretized, thus reducing the spatial dimension by one. As a result of the semi-discretization process, a set of ordinary differential equations is obtained, which can be solved analytically to obtain the static stiffness matrix. The SBFEM is applicable to bounded and unbounded domains. Since locking effects are largely affected by the thickness of the structure, it is expected that discretizing only the mid-surface and handling the solution analytically in the through-thickness direction might decrease locking effects. The development of plate elements based on the SBFEM has already demonstrated that the proposed semi-analytical approach completely avoids shear locking, which occurs for thin plates. Thus, the SBFEM seems to be a promising method to model shell structures with reduced locking effects.
First studies such as a simplified plane strain arch formulation to approximate an axisymmetric cylindrical shell will be presented. This approximation already shows a high correlation with the membrane theory of shells. Furthermore, first results obtained for 3D shell formulations will illustrate the potential of the proposed approach based on the SBFEM.

Automatic quadtree-based modeling using a coupled SBFEM/SCM approach

H. Gravenkamp (University of Duisburg-Essen), S. Duczek (Otto-von-Guericke-University of Magdeburg), C. Birk (University of Duisburg-Essen) 16:50

The quadtree decomposition is often recognized as a highly efficient way to discretize arbitrary geometries, particularly in the context of automatic image-based simulations. A typical quadtree discretization consists of square-shaped cells only, while each square can successively be subdivided into four quadrants depending on the inhomogeneities

or gradients that need to be resolved. Unfortunately, this strategy is not applicable to conventional finite element implementations in a straightforward fashion without introducing hanging nodes at the interfaces between elements of different size. It has been demonstrated recently that the scaled boundary finite element method (SBFEM) can directly exploit quadtree meshes since in this method only the boundaries of each cell need to be discretized by an arbitrary number of line elements. The SBFEM offers the additional advantage that the order of interpolation can be chosen individually for each subdomain, depending on its size and material parameters.
On the other hand, the convergence of quadtree-based methods can be poor due to the introduced geometry error. Considering structures with complex curved boundaries, a staircase representation of the boundary is often insufficient. To overcome this drawback, the quadtree-based SBFEM is coupled with the spectral cell method (SCM) to capture the modeled geometry more accurately. The SCM is a fictitious domain method that is usually defined on a regular structured finite element mesh. Rather than modifying the shape of each element through adequate mapping, the geometry is considered during the integration of the stiffness and mass matrices. In the proposed approach, the SCM concept is only employed for the smallest cells of the quadtree decomposition to obtain a smoothed and more realistic approximation of the actual geometry. That is to say, all cells that are intersected by the physical boundary of the computational domain are treated in an SCM-sense, while all other cells are computed as SBFEM subdomains. This methodology minimizes the required number of degrees of freedom and avoids the need for a two-dimensional quadrature in all cells that do not contribute to the approximation of the boundary. Numerical examples include static image-based analyses of complex geometries and the simulation of wave propagation phenomena in strongly inhomogeneous domains.

Nonlinear analysis of solids in boundary representation - a NURBS based Galerkin method

M. Chasapi (RWTH Aachen University), B. Simeon (Technische Universität Kaiserslautern), S. Klinkel (RWTH Aachen University) 17:10

The contribution presents a new numerical method to solve nonlinear problems of solids in boundary representation. A formulation for material nonlinearities is derived. The proposed method introduces an approach where the geometrical description of the boundary is sufficient to define the complete solid. While the interior of the domain is described by a radial scaling parameter, the scaling of the boundary with respect to the specified scaling center leads to the complete solid. This idea fits perfectly to the boundary representation modeling technique commonly employed in CAD. The approach exploits the tensor-product structure of the solid to parameterize the physical domain, i.e., two-dimensional surfaces are represented by NURBS objects, which parameterize the boundary surfaces. Following the isogeometric paradigm, the NURBS functions that describe the boundary of the geometry form also the basis for the approximation of the displacement at the boundary. The displacement response in the circumferential and radial scaling direction is approximated by one-dimensional NURBS. The present formu-

lation accounts for material nonlinearity with elasto-plastic behavior, where small strain theory is assumed. Similar to the Scaled Boundary Finite Element Method (SB-FEM), the structure is parameterized by a radial scaling parameter that emanates from a scaling center and a parameter in circumferential direction along the boundary. The Galerkin projection of the weak form yields a system of equilibrium equations whose solution gives rise to the displacement response. Due to the nonlinear relation between the stress and the strain, the linear equilibrium equation is not applicable anymore. Applying the weak form in the circumferential and radial direction leads to a nonlinear equation with respect to the unknown displacement response, which is solved with a linearization and the Newton-Raphson scheme. The applicability of the proposed formulation is shown by means of numerical examples.

A guideline procedure to conduct the divide mesh in scaled boundary finite element method

Y. Khudari bek (Bauhaus-Universität Weimar), C. Könke (Bauhaus-Universitaet Weimar) 17:30

The scaled boundary finite element method (SBFEM) is a semi-analytical method developed by Song and Wolf[1, 2]. It is highly efficient in solving problems involving singularities, and it is a unique novel to solve unbounded domain problems. In SBFEM, the discretization technique, which is applied in the circumferential direction, has a significant influence on the accuracy of the solution. However, using a large number of nodes on the boundary increases the computational effort, because it includes the solution of a quadratic Eigenvalue problem. Sub-structuring in SBFEM has an interesting feature to analyze material variation and geometry in the problem. In this study a guideline mesh procedure is introduced based on comparison between boundary discretization for sub-domains and including additional sub-domains. Then the unique discretization level is chosen depending on the accuracy and computational time. Different levels of discretization for the sub-domains are proposed and compared with uniform sub-structuring, h-adaptive SBFEM and FEM. Two benchmark examples introduced to investigate the proposed algorithm. The output showed high efficiency and produced an effective tool to analyze the problems that need sub-structuring in SBFEM.

[1] C.Song and J.Wolf, The scaled boundary finite-element method—alias consistent infinitesimal finite-element cell method—for elastodynamics 147, page (1997).

[2] J.Wolf and C.Song, The scaled boundary finite-element method–a primer: derivations 78,(2000).

Stress solutions for joints with nonlinear adhesives

P. Rosendahl (Technische Universität Darmstadt), N. Stein, W. Becker (Technische Universität Darmstadt) 17:50

Simple, efficient predictive models are valuable tools in the structural design process of adhesive joints, in particular for quick assessments in early stages. There is a rich

history of stress solutions for adhesive joints which model the adhesive as smeared linear elastic springs [1–3], also known as weak interface, spring-type interface or imperfect interface models. Such models provide excellent results for sufficiently brittle adhesives. However, rubber-modified epoxies or silicone adhesives exhibit nonlinear behavior even under small loadings. Nonlinearities can for example arise from hyperelastic characteristics or plasticity. In particular the stress concentrations at the overlap ends are prone to trigger local nonlinear effects. The present work outlines a simple load transfer model for joints with hyperelastic or elasto-plastic adhesives.
The present model considers the overlap region as a sandwich-type element under general loading, similar to the linear-elastic models by Bigwood and Crocombe [4] or Weißgraber et al. [5]. Considering the overlap only, allows for investigation of arbitrary joint geometries such as single lap joints, double lap joints, reinforcement patches, T-joints, L-joints or corner joints. The boundary conditions, i.e. section forces and moments can be derived from linear statics or other adequate methods. The adhesive is represented by an infinite set of nonlinear springs. Constitutive equations for the adhesive are derived for both, hyperelastic and elasto-plastic materials in plane strain state. For hyperelastic materials, nearly incompressible behavior with no restriction regarding the choice of strain energy density function is modeled. The constitutive properties of elasto-plastic adhesives are described by deformation theory of plasticity.
A thorough comparison with finite element analysis (FEA) reveals a good agreement of the shear and peel stresses predicted by the present model and FEA. The model is tested for a number of different joint geometries and material combinations. Limits of the applicability of the present model are extracted. However, the stress solution is rendered well for a wide range of parameters and elasto-plastic or hyperelastic adhesives.

[1] O. Volkersen. Die Nietkraftverteilung in zugbeanspruchten Nietverbindungen mit konstanten Laschenquerschnitten. *Luftfahrtforschung* 15(1/2):41–47, 1938.

[2] M. Goland, E. Reissner. The stresses in cemented joints. *Journal of Applied Mechanics* 11(1):A17–A27, 1944.

[3] I. Ojalvo, H. Eidinoff. Bond thickness effects upon stresses in single-lap adhesive joints. *AIAA Journal* 16(3):204–211, 1978.

[4] D. A. Bigwood, A. D. Crocombe. Elastic analysis and engineering design formulae for bonded joints. *International Journal of Adhesion and Adhesives* 3(11):229–242, 1989.

[5] P. Weißgraeber, N. Stein, W. Becker. A general sandwich-type model for adhesive joints with composite adherends. *International Journal of Adhesion and Adhesives* 55:56–63, 2014.

An application of double collocation point approach in terms of the Boundary Element Method to plate analysis

M. Guminiak (Poznan University of Technology), J. Wierzbicki (Adam Mickiewicz University) 18:10

The Boundary Element Method (BEM) can be applied in the wide aspect of static, dynamic and stabilty analysis of structures [1], [2], [3]. The thin plate bending is described by two boundary (static analysis) [4] and boundary-domain integral equations (dynamic and stability analysis) [4], [5], [6]. In present paper static and dynamic analysis of Kirchhoff plates of any shape are considered. Additonally the stability anaylsis of rectangular plates is carried out. The direct approach of the BEM with static fundamentalo solution are applied. The constant and parabolic type of boundary element are introduced. Governing equations are formulated in singulat and non-singular term using single and double collocation point approach [7], [8]. To carrying out the stability analysis, the plate domain is divided into finite number of rectangular sub-domains having character of plane elements of the constant type. Inside each of them the curvature is defined at the central collocation point. The curvature can also be established by application of simple difference operators constructed using deflections at the central and neighbouring collocation points. External in-plane loading has the conservative character. The boundary and boundary-domain integral equations are formulated in simplified form without introducing Kirchhoff forces: corner concentrated forces and equivalent shear force along simply-supported edge. Along an edge free, the angle of rotation in tangent direction is expressed by simple difference operator constructed using deflection established at two neighbouring field points. Analysed numerical examples demonstrate the sufficient effectiveness of the proposed approach.

[1] Burczyński T., The Boundary Element Method in Mechanics, Technical-Scientific Publishing house, Warszawa, 1995 (in Polish). [2] Wrobel L.C., Aliabadi M.H., The Boundary Element Methods in Engineering, McGraw-Hill College. ISBN 0–07–707769–5, 2002. [3] Katsikadelis J.T., Sapountzakis E.J., Zorba E.G., A BEM Approach to Static and Dynamic Analysis with Internal Supports, Computational Mechanics, 7(1), pp. 31–40, 1990. [4] Guminiak M., Static and Free Vibration Analysis of Thin Plates of the Curved Edges by the Boundary Element Method Considering an Alternative Formulation of Boundary Conditions, Engineering Transactions, 64, 1, 3—32, 2016. [5] Guminiak M., Sygulski R., Vibrations of system of plates immersed in fluid by BEM, Proceedings of IIIrd European Conference on Computational Mechanics, Solids, Structures and Coupled Problems in Engineering ECCM-2006, pp. 211, eds.: C.A. Mota Soares, J.A.C. Rodrigues, J.A.C. Ambrósio, C.A.B. Pina, C.M. Mota Soares, E.B.R. Pereira and J. Folgado, CD enclosed, June 5–9, 2006, Lisbon, Portugal. [6] Guminiak M., An Alternative Approach to Initial Stability Analysis of Kirchhoff Plates Resting on Internal Supports by the Boundary Element Method, Engineering Transactions, 63, 3, 273—296, 2015. [7] Guminiak M., An Alternative Approach of Initial Stability Analysis of Kirchhoff Plates by the Boundary Element Method, Engineering Transactions, 62(1), pp. 33–59, 2014. [8] Wierzbicki J., Static of Kirchhof plates by the Boundary Element Method using double collocation point approach (in Polish), Engineering thesis, Poznan

University of Technology, Institute of Structural Engineering, 2016.

S 4 : Structural mechanics

Friday 09:00 - 11:00 Marienstr. 13, Ground floor, Lecture hall C

Nonlocal balance of angular momentum from stress field analysis

I. Münch (KIT) 09:00

For simple materials Noll's principle of local action yields the stress tensor function to depend only on the local deformation gradient or its history. Consequently, the stress field is of class $\mathbb{C}^1$. Couple stress theories drop the principle of local action and account for higher gradients in deformation or introduce additional kinematical variables, respectively. Then, the stress tensor field in the contiguity of a continuum point can become a nonlinear function. Consequently, power series expansion of stress needs higher order terms in the representative volume element around the continuum point. We axiomatically consider the stress field tensor as nonlinear function of class $\mathbb{C}^2$, approximated via power series expansion of order two from the midpoint of a cubic representative volume element. Depending on the grade of approximation, the series expansion reproduces nonlinearities of the stress field in the cube and also on its surface. The proposed procedure yields an algebraic formula for the couple stress tensor with an internal length scale parameter. It evolves from integrating couples from tractions on the surfaces of the cube. The resulting couple stress tensor is isotropic and frame invariant. Consequently, it inherits properties of the stress field, e.g. symmetric stress yields trace free couple stress. Note, that no use of Green's divergence theorem is made. The approach is not restricted by material constitution such that it is valid for solids and fluids. At least it is found that the nonlocal balance of angular momentum incorporates the curl of the stress field. The proposed equations can help to evaluate nonlocal continuum models.

Advanced Rebar Formulation within a Thermo-Mechanically Coupled Tire Simulation

T. Berger (Institut für Statik und Dynamik der Tragwerke, TU Dresden),
M. Kaliske (TU Dresden) 09:20

As shown in various experiments, coupling between the thermal and the mechanical field of a rolling tire in contact with a rigid surface can be observed. An increase of its temperature over time when rolling with a constant velocity can be seen. This phenomenon is caused by the viscoelastic material properties, where the dissipated energy will lead to a heating of the rubber. Also the constitutive behaviour will change, when the temperature increases. A nonlinear viscoelastic material model is chosen to model an amplitude dependency of the time dependent behaviour of the rubber, proposed by Bergström and Boyce [1].
Another important part of a tire are the reinforcements, which are embedded inside the

rubber. These consist mostly of steel or polyester. These materials are not known for a dissipative behaviour and will not contribute to the heating of the tire. However, they also change their properties with increasing temperature and have a significant influence on the overall tire properties. Even without a contribution to the heating, the reinforcements will change its conductivity and have to be taken into account.
For an accurate and efficient way to model the thermo-mechanical coupling, an in-house framework [2] will be presented, by use of the Arbitrary Langrangian Eulerian formulation and the commercial code ABAQUS [3]. It is assumed, that the temperature in circumferential direction will stay constant and instant coupling effects are negligibly small. Therefore, the problem is split into a thermal and a mechanical part, and the coupling quantities (dissipated energy and temperature) are updated in a sequential manner.
A common practise to model the reinforcements in tires is to use smeared layers, which leads to some difficulties. First of all, the modelling is only valid for a really small spacing between the bars. Another problem is, that in ABAQUS, the heat transfer algorithm will omit any embedded elements. Because of that, the mesh has to be refined, which leads to an increasing computation time and can cause numerical difficulties, due to too small elements.
In this contribution, a different way of modelling the rebars within a thermo-mechanical coupled algorithm is presented without the assumption of a smeared layer and treat them as single rebars. In numerical examples, the advantages of the proposed method are presented and the difference to the classical approach is shown. Also, the influence of the reinforcements on the stiffness, heat generation and rolling resistance of the tire, will be discussed.

[1] J.S. Bergström, M. Boyce, Constitutive modeling of the large strain time-dependent behavior of elastomers, Journal of the Mechanics and Physics of Solids 46 (1998) 931-954.

[2] R. Behnke, M. Kaliske, Thermo-mechanically coupled investigation of steady state rolling tires by numerical simulation and experiment, International Journal of Non-Linear Mechanics 68 (2015) 101-131.

[3] Dassault Systèmes (Ed.), Abaqus 6.14-EF Online Documentation, 2014.

Comparison between Substructure and FE² modeling of beam-like structures

S. Klarmann (Technische Universität Darmstadt, Fachgebiet Festkörpermechanik), F. Gruttmann 09:40

Beam elements are a powerful tool to model large structures which possess beam-like behavior. To perform those calculations, the most essential part are effective material properties. Different approaches are possible to obtain these, like in [1]. An extension to take inhomogeneities in length direction of the beam into account, can be done with the FE^2 scheme like in [2]. This approach has the drawback of a length dependency of the shear stiffness, resulting from the double fulfillment of the equilibrium condition.

A more flexible way to overcome those problems is the substructure modeling. Beam elements are perfectly suited for this approach because of their 1D geometrical characteristic. The most essential part is to reduce the cross-section to a point with beam-like kinematics. Like in the FE^2 approach, the application of suitable boundary conditions is necessary.
This work aims at the comparison between substructure and FE^2 modeling of beam-like structures. It is worth mentioning that the steps of a calculation within the substructure approach are the same as in FE^2. Both cases will be compared with suitable numerical examples.

[1] F. Gruttmann, R. Sauer and W. Wagner. Theory and numerics of three-dimensional beams with elastoplastic material behaviour. Int. J. Numer. Meth. Engng. 48 (2000) 1675–1702.

[2] F. Gruttmann, W. Wagner. A coupled two-scale model with applications to layered structures. Int. J. Numer. Meth. Engng. 94 (2013), 1233–1254.

The Finite Cell Method: Polygonal and Tetrahedral Cells

S. Duczek (Otto-von-Guericke University Magdeburg), U. Gabbert (Otto von Guericke University Magdeburg) 10:00

Today, the Finite Element Method (FEM) is the dominant numerical tool for solving Partial Differential Equations (PDEs). The widespread use of this particular method is based on its flexibility to describe arbitrary geometries and on its ability to handle classes of problems. It suffers, however, from the need for body-fitted discretizations and therefore the mesh generation process is often regarded as the bottleneck in the simulation process. The discretization both requires a significant input by the user and is rather error-prone. One idea to circumvent or at least alleviate this drawback is to employ the Fictitious Domain Concept (FDC) which provides a simplified meshing strategy based on Cartesian grids. In conjunction with higher order shape functions, known from the *p*-version of the FEM, the method is commonly referred to as the Finite Cell Method (FCM).
So far, the FCM has only been used in connection with structured quadrilateral (2D) and hexahedral (3D) meshes and therefore, it is the main goal of the current contribution to illustrate possibilities for an extension to unstructured grids. In two-dimensional cases, polygonal finite elements based on generalized barycentric coordinates are deployed, while in three-dimensional applications tetrahedral elements are the preferred choice.
The main advantage of the proposed polygonal approach (2D) is that it inherits the ability of polygonal finite elements for a local mesh refinement and for the construction of conforming quadtree meshes (without introducing hanging nodes). In the tetrahedral approach (3D) an important benefit is the possibility to re-use finite element grids from commercial FEM pre-processors. These meshes can be easily transferred to the FCM and only important micro-structural details need to be included by deploying the FDC. Such an approach is especially advantageous for highly heterogeneous cellular materials.

To this end, the geometry of the micro-structure is obtained by means of computed tomography (CT) where only the parts of interest are scanned with high resolution computer tomographs. These CT-scans can be included in the FCM model in two ways: (*i*) directly using the voxelized data or (*ii*) further processing the data and generating surface tessellation language (STL) files to describe the boundary of the micro-structure. The performance of both unstructured FCM versions are illustrated by means of several benchmark problems.

Investigation of strain-rate effects in Al foams and Ni/Al hybrid foams on different scales

A. Jung (Universität des Saarlandes), J. Luksch, M. Felten, D. Sory (Imperial College), A. Pullen (Imperial College), W. Proud (Imperial College), M. Larcher (European Commission, JRC Ispra), G. Valsamos (European Commission, JRC Ispra), G. Solomos (European Commission, JRC Ispra) 10:20

Open-cell metal foams are a relatively new class of cellular materials with structural features resembling to lightweight load-bearing materials such as cancellous bones and wood. Their high stiffness-to-weight ratio coupled with their typical long flat stress-strain make them ideal candidates as cost-effective shock energy absorbers, e.g. in the case of car crash, against bird strike or blast. The macroscopic mechanical properties of foams are strongly influenced by both the mechanical behaviour of single pores at the mesoscopic level and the struts and their structure at the microscopic length-scale based on a strong structure-property relationship.

Ni/Al hybrid foams are a type of open-celled materials consisting of an aluminium substrate foam coated with nanocrystalline nickel, which strengthens the struts leading to significantly improved global properties such as a tenfold energy absorption capacity compared to pure aluminium foams [**?**]. The mechanical properties of the Ni/Al hybrid foams can be tailored by the coating thickness and coating properties, which make Ni/Al hybrid foams a multifunctional material. Although metal foams are in general used in dynamic applications, they are mainly characterised under quasi-static loading conditions.

The aim of this study is to report an experimental-numerical procedure to investigate the strain rate-dependent effects of Ni/Al hybrid foams arising in individual struts, individual pores as well as in macroscopic specimens. This is of importance to understand the structural influence on strain rate-dependent material properties such as energy absorption capacity in these kind of foams and improves the design of foam-based components. Uniaxial compression tests were performed from quasi-static to high strain rate using a standard mechanical testing, drop-weight rigs and high-velocity impact gas gun. A novel method based on photogrammetry was used to generate real geometry finite element micromodels of the individual pores. Numerical calculations using a Johnson-Cook model outlines microinertia effects arising from the pore geometry along with strain rate-behaviour associated to the nickel coating in Ni/Al hybrid foams.

[1] A. Jung et al. Nanonickel coated aluminum foam for enhanced impact energy absorption. Adv. Eng. Mater., 2011, 13, 23-28

Smart and functionally graded structures: Variational-asymptotic approach and error estimation

K. Le (Ruhr Universität Bochum) 10:40

An asymptotically exact two-dimensional theory of functionally graded piezoelectric shells is derived by the variational-asymptotic method. The error estimation of the constructed theory is given in the energetic norm. As an application, analytical solution to the problem of forced vibration of a functionally graded piezoceramic cylindrical shell with thickness polarization fully covered by electrodes and excited by a harmonic voltage is found.

S 4 : Structural mechanics

Friday 11:30 - 13:30 Marienstr. 13, Ground floor, Lecture hall C

Local buckling of laminated composite beams based on different plate theories

J. Herrmann (Helmut Schmidt University / University of the Federal Armed Forces Hamburg), T. Kühn (EADS EFW – Elbe Flugzeugwerke), T. Müllenstedt (Helmut Schmidt University / University of the Federal Armed Forces Hamburg), S. Mittelstedt (SOGETI Deutschland GmbH), C. Mittelstedt (TU Darmstadt) 11:30

The present paper deals with the onset of local buckling of compressively loaded thin-walled beams made of orthotropically laminated composite materials using discrete plate analysis. The analysis model focusses on the buckling of webs and flanges of composite beams with arbitrary cross-sections under uniform longitudinal compressive load. In order to account for transverse shear deformations as they are typical for moderately thick to thick laminated composite materials made of e.g. carbon fibre reinforced plastics, the present analysis is based on various laminate plate theories. The idealisation consists of modelling the webs as being simply supported at all four edges, while at the longitudinal unloaded edges an elastic clamping is assumed which is represented by a clamping stiffness that takes material, geometry and layups of the adjacent flanges of the beams into account. Accordingly, the flanges are treated as plates with three simply supported edges and one free edge, wherein the unloaded simply supported edge is elastically clamped in order to represent the rotational support by the adjacent web. The analysis of the web and flange buckling loads is performed using the Rayleigh–Ritz-method employing specifically chosen shape functions for the out-of-plane displacements and the rotations of the cross-sections. The accuracy of the employed approaches is established by comparison with accompanying finite element simulations of actual

thin-walled composite beams. It is revealed that the presented methodology is highly efficient in terms of computational effort and yet performs with satisfying accuracy which makes it very attractive for actual practical applications whenever the local stability behaviour of composite beams is to be considered.

FE-Simulation based analyses of strain localizations in an ECAP process

T. Horn (TU Chemnitz), C. Silbermann (TU Chemnitz), P. Frint (TU Chemnitz), J. Ihlemann (TU Chemnitz) 11:50

Equal-channel angular pressing (ECAP) is an attractive processing method to introduce large plastic strains into different materials, which often results in an ultrafine-grained microstructure. In several cases there exist distinct strain localizations, whose principle is not fully understood. Frint [1] termed these localizations shear bands and the regions between them matrix bands.

In this contribution, FE-simulations of the ECAP process and corresponding analyses are presented. The material behavior is modelled by the continuum-mechanical, phenomenological material model of Shutov & Kreißig [2]. It will be shown that localizations can be simulated with accurate correspondence to the experimental results of Frint [1]. Moreover, an analysis of the influence of the material parameters showed that the kinematic hardening has a prominent role to the simulation of the localizations.

As conclusion of his experimental investigation, Frint [1] formulated a model concept for the development of the shear bands. This concept was evaluated and extended by the help of FE-simulations. In contrast to Frint, plastic deformations are observed not only in the shear but also in the matrix bands. Further, a detailed stress-strain analysis during ECAP was conducted, which leads to a better understanding of the shear and matrix band evolution of the metal.

[1] P. Frint, *Lokalisierungsphänomene nach kombinierter hochgradig plastischer Umformung durch Extrusion und ECAP einer 6000er-Aluminiumlegierung*, Dissertation, Chemnitz University of Technology, 2015
[2] A. Shutov, R. Kreißig, *Finite strain viscoplasticity with nonlinear kinematic hardening: Phenomenological modeling and time integration*, Computer Methods in Applied Mechanics and Engineering, pp. 2015-2029, 2008

Simulation of the Presta joining process - Transfer of the deformation history between the single simulation steps

R. Scherzer (Chemnitz University of Technology), C. Silbermann (Chemnitz University of Technology), J. Ihlemann (Chemnitz University of Technology) 12:10

The Presta joining process is the world's leading manufacturing method for assembled camshafts. It is a multi-stage forming process separated in different steps. First, the rolling of the shaft creates a local widening of the intended cam seat. Within the subsequent joining process, the cam is forced onto the widened cam seat to form a tight

fit. In these processes large local deformations occur, which requires an appropriate material model. The phenomenological material formulation of finite strain viscoplasticity implemented in the introduced simulation model enables the transfer of the deformation history to a new reference configuration. Hence, at the change of simulation models this feature is applied by passing the material model's internal state variables of the rolling step to the initial FE-mesh of the joining step. This work shows the simulation models of the Presta joining process and gives a detailed insight into the change of the reference configuration.

Investigations on a FEM-sub-model for "Die-Less-Hydroforming" weld-seams

A. Metzger (Karlsruher Institut für Technologie (KIT)), D. Ruff (Karlsruher Institut für Technologie (KIT)), T. Ummenhofer (Karlsruher Institut für Technologie (KIT)) 12:30

The special forming process called "Die-Less-Hydroforming" is very up to date among many users from academic research, industrial (prototypical) applications, arts and design as well as some hobbyists. During "Die-Less-Hydroforming" at least two steel blanks are joined at the edges of the blanks by welding with a circumferential seal weld. A two-dimensional flat "envelope" made of thin steel sheets results, that is formed into a spatial structure by inflating it with a pressurized medium, e.g. water.
A global FE-simulation of this forming process with LS-DYNA was already developed and presented by the authors (see [1] and [2]). Weld seams executed as edge welds are used here. These weld seams have to be carried out as filigree as possible (in the type of a linear flow zone) to enable a good formability. At the same time, they should not tear open until the end of plastic deformation and should stay sealed. The high local plastic strains in the weld seam pose a special major challenge to those and to the related welding process.
When looking to the global forming simulation FE-model for "Die-Less-Hydroforming" in recent publications [1] and [2], the blanks are discretized by Belytschko-Tsay-shell elements and –as a special modeling step– the seal weld is modeled by merging the duplicated nodes in the welded joining zone. In this contribution some results of a structure-mechanical FE-sub-model of this special weld seam are presented, in order to verify the kind of modeling of the weld seam in the global FE-model of "Die-Less-Hydroforming". In detail, the load-displacement-performance and stiffness behavior of the weld-seam model and the correspondence with the real behavior is investigated. Especially for this, a practical combined bending-tension-test for the investigation of these weld seams was developed at our institute. In addition, this test easily allows assessing the suitability, the quality and the formability of a weld seam for "Die-Less-Hydroforming".
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Less-Hydroforming-Structures", Proc.Appl.Math.Mech.15, 215–216, doi:10.1002/pamm.201510098

Deformation analysis of Mg bending specimens using Digital Image Correlation

T. Lehmann (Chemnitz University of Technology), J. Müller (Chemnitz University of Technology), J. Ihlemann (Chemnitz University of Technology) 12:50

This contribution deals with the determination and evaluation of displacement fields of Mg (AZ31 TRC) bending specimens using Digital Image Correlation (DIC) technique. The bending tests were performed at temperatures of 250 and 350 °C. The experimental setup includes a special bending device which is assembled in a testing machine. Both the bending device and the specimen are surrounded by a temperature chamber. By means of DIC the in-plane displacement fields at the surface of the specimens were determined. The evaluation of the DIC data was performed with MATLAB. Polynomial and smoothing spline approximation were used to smooth the experimental displacement fields and to get mathematical functions for determination of Hencky strains as well. A comparison of the two different approximation methods is demonstrated. The deformation analyses will be used for verification of numerical simulations of the bending tests.

S 5: Nonlinear oscillations

Organizers: Hartmut Hetzler (University of Kassel)
Dieter Lens (GSI Helmholtzzentrum für Schwerionenforschung)

S 5 : Nonlinear oscillations

Tuesday 14:00 - 16:00 Marienstr. 7, 2nd floor, Room 206
Chair: Hartmut Hetzler (Universität Kassel)

Optimization of Damping for Squeal Avoidance in Disc Brakes

D. Jekel (TU Darmstadt), P. Hagedorn (TU Darmstadt) 14:00

In mechanical engineering, self-excited vibrations are a frequent and unwanted occurrence. An example of this phenomenon is the squealing of automotive disc brakes, which is due to friction between the brake disc and the brake pads [1]. It is well known, that such systems are very sensitive to damping and that their stability behavior may strongly depend on the structure of the damping matrix [2]. Although these problems are inherently nonlinear, a standard stability analysis approach involves linearizing the equations of motion around an equilibrium, which results in a system of second order

linear differential equations of the form

$$\mathbf{M}\ddot{\mathbf{q}} + (\mathbf{D} + \mathbf{G})\dot{\mathbf{q}} + (\mathbf{K} + \mathbf{N})\mathbf{q} = \mathbf{0}, \tag{6.1}$$

where $\mathbf{q} \in \mathbb{R}^n$ is the column vector of the generalized coordinates and the dots stand for differentiation with respect to time. In most technically relevant applications, the mass matrix $\mathbf{M}$ and the stiffness matrix $\mathbf{K}$ are symmetric and positive definite, while the gyroscopic matrix $\mathbf{G}$ and the circulatory matrix $\mathbf{N}$ are skew-symmetric [3]. The damping matrix $\mathbf{D}$, which is symmetric and in nearly all applications is at least positive semi-definite, is the focus of this study.
For the formulation of an optimization problem and to account for the different physical origins, the damping matrix $\mathbf{D}$ of (6.1) can be written as a linear combination

$$\mathbf{D} = \mathbf{D}_0 + \sum_{j=1}^{k} \alpha_j \mathbf{D}_j, \tag{6.2}$$

where $\mathbf{D}_0$ is a matrix containing fixed damping terms and $\mathbf{D}_j$ are α_j-weighted damping matrices whose relative contribution to the overall damping is to be varied. Thus, the different physical damping mechanisms occurring in disc brake models, e.g. viscous damping, friction induced damping, and material damping, can be treated independently. Using standard complex eigenvalue analysis and a form of the damping matrix according to (6.2), the stability of (6.1) can be optimized by varying the weighting factors α_j in order to either stabilize or make more stable the equilibrium state subject to sensible constraints. For this purpose, a system is considered to be more stable if its eigenvalue with largest real part is as small as possible.
In this presentation, we apply the optimization technique outlined in [4], where a minimal model of a disc brake with only two degrees of freedom was studied. The main goal is to extend these findings to a more realistic, high dimensional finite element brake model which is also used in industry. To this end, modal reduction techniques as well as Matlab's optimization toolbox are used.

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Investigation of Vibrations Induced by Dry Friction in a Pin-on-Disk Experimental Set-up

S. Kapelke (Karlsruher Institut für Technologie), L. Oestringer, W. Seemann (Karlsruher Institut für Technologie) 14:20

High-frequency vibrations have been shown to smooth the effective characteristics of dry friction and may be used in order to quench undesired phenomena such as friction induced vibrations. This effect of vibrational smoothing has been subject of numerous publications in the past and is used successfully in several industrial applications. As the agreement between classical modelling and related experimental results appears to be insufficient, the effect of contact compliance on vibrational smoothing of dry friction has been discussed. Using a class of dynamic friction models, the effective friction-velocity characteristics of a simple 1-DoF friction oscillator have been presented. Recently, a pin-on-disk experimental set-up has been developed in order to validate the corresponding results. Within this contribution, selected properties of the experimental set-up are analysed. Due to a negative slope in the friction-velocity characteristics, friction induced vibrations can be observed at low sliding velocities. The oscillatory behaviour of a corresponding minimal model is investigated and compared to the experimental results. When applying appropriate high-frequency excitation, the friction-velocity characteristics are smoothed and, consequently, friction induced vibrations can be quenched. The experimental results are compared to those obtained for an elasto-plastic friction model.

On the electromechanical coupling in rotordynamics of electrical machines

F. Boy (University of Kassel), H. Hetzler (University of Kassel) 14:40

The assessment of oscillations in the context of rotordynamics caused by electromechanical interactions in electrical machines has been a major field of research within the last decades. The discussion includes reliability and noise issues [1, 2], as well as online system state monitoring [3]. From a general point of view, models of electrical machines comprise three subproblems: As a first point it is necessary to describe the mechanical part in terms of torsional- and lateral bending vibrations of the rotor, possibly combined with the deformation of the stator housing. Furthermore, there are several electrical circuits, which are diverse in their design, but can basically be described by ordinary differential equations. These both parts interact through the magnetic field, which is caused by the flowing currents and affected by the mechanical motion.
Obviously a proper description of electromechanically induced oscillations demands for an adequate modelling approach, including the mechanical- and electrical degrees of freedom as well as a proper way to handle the nonlinear magnetic field problem. Certainly, there are a lot of different ideas to treat the problem and all of them have their advantages and drawbacks, when it comes to the assessment of vibrations in the context of nonlinear rotordynamics. At the one hand side, there are analytical methods (e.g. [1, 4, 5]), which offer the possibility to get a clear insight into parameter dependencies and the involved physics but lack an adequate description of the magnetic field problem. More recent numerical methods (eg. [6, 7]) in contrary are inverse to that.
This contribution is devoted to providing a critical discussion on established modelling

approaches and their applicability for dynamical analysis. The considerations decribed here are based on an integrated approach based on the electromechanical Lagrange's Equations of second kind. It turns out that especially the basically well suited analytical methods often imply assumptions, which may strongly affect the prediction of oscillations. This fact is demonstrated for the simple example of an cage induction machine. Here it can be seen, that neglecting motional induction completely changes the prediction of self excited oscillations. As a consequence the question is posed, whether it is possible to overcome the known difficulties either by improving one branch of methods, or by combining them.

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A quasi-axisymmetric lattice model applied to analyze the vibrational contact between a PTFE shaft seal and a rotor

F. Albrecht (HAW Hamburg), T. Kletschkowski (HAW Hamburg) 15:00

Shaft seals are used to prevent leakage of oil and intrusion of dirt particles at rotating machineries. The contact pressure between seal and shaft is essential to ensure the functionality of a sealing system. It must be designed for the most critical operating points and therefore leads to unnecessary wear and frictional losses at all other conditions. An adaptive seal with adjustable contact pressure could be used to avoid such problems. In order to analyze different active and passive designs for such a seal, transient

thermo-mechanic simulations considering highly nonlinear visco-plastic material behavior at finite strains as well as non-linear contact between shaft and seal are required. To reduce the complexity as well as to increase the computational efficiency, the seal is discretized with a quasi-axisymmetric lattice structure consisting of bar elements and discrete mass points. This locally one dimensional approach allows a direct implementation of a visco-plastic rheological model for PTFE. The elastic shaft is described by a Laval-Rotor. An implicit time-domain integration scheme is used to solve the equations of motion of the coupled system shaft-seal and to calculate the radial distribution of the contact pressure. The results show a good followability of the seal for low rotor speeds. At very high speeds, the followability of the seal is not sufficient. This is also confirmed by the results of a numerical modal analysis. Thus, an adaptive mechanism would be needed to prevent leakage effects. To analyze such mechanisms that could be based on shape memory effects, it will be necessary to include frictional heat generation, heat conduction and aspects of wear in the simulation model. This is part of upcoming work.

Rotor-systems with compliant seals: A comparison of the rotordynamics using the Muszynska model and Hirs' lubrication equations

S. Bäuerle (University of Kassel), H. Hetzler (University of Kassel) 15:20

Compliant seals offer a comparatively new design approach combining low leakage and low wear properties (e.g. Gland-seal [1], Halo-seal [2]). These advantages can be achieved by a narrowed seal gap along with added flexibility lowering the risk of rotor-seal rubbing.
Our main interest is to investigate the influence of compliant seal properties on rotor dynamics. Therefore, a model consisting of a *Laval*-rotor (or *Jeffcott*-rotor) and a visco-elastically supported stiff seal ring has been set up. Previous investigations [3] show an enlarged stable operation range. Rotor vibrations occurring after a loss of steady state stability were small so that an ongoing operation might be possible.

In this contribution two modelling approaches for the fluid forces are compared: the previously used parametric *Muszynska*-model [4] defines non-linear ODEs in dependence of rotor and seal deflection. The parameters are fitted for the present case using *Childs* analytic formulas [5].
The second approach under consideration are *Hirs'* PDEs for the description of turbulent lubrication flow [6]. Here, the radial flow component and every radial dependencies are neglected due to the comparatively small sealing gap. The influence of the turbulent flow characteristics is modelled semi-empirically. On the one hand, these equations are numerically integrated in order to obtain rotordynamic coefficients for an ODE model. These coefficients depend on rotor and seal deflection as well as on the rotational speed of the rotor. On the other hand, a fully coupled model of the rigid body movement of rotor and seal as well as the fluid film description by *Hirs'* is set up.
The investigation compares the coefficient model of *Muszynska* with the one obtained by integrating *Hirs'* equations with an emphasis on the non-linear behaviour. The predictions made by using these two models are then contrasted with the ones made by the

fully coupled model. Run-up simulations for an unbalanced rotor are carried out and the non-linear behaviour of a balanced rotor is considered.

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A Minimal Dynamic Structure Model Considering Dry Friction Energy Dissipation in Gas Foil Bearings

T. Leister (Karlsruhe Institute of Technology), S. Bard (Karlsruhe Institute of Technology), W. Seemann (Karlsruhe Institute of Technology) 15:40

During the last few decades, successful applications of gas foil bearings (GFBs) in air cycle machines of commercial aircraft have confirmed the remarkable potential of this technology in the light of an increasing demand for energy-efficient turbomachinery. Besides excessively low wear and power loss due to the absence of solid-to-solid contact between the airborne rotor journal and the bearing sleeve, the use of GFBs permits to overcome yet insurmountable speed, temperature, size, weight, and cleanliness limitations of conventional rolling-element bearings. However, most GFB rotor systems are prone to undesirable self-excited vibrations with comparatively large amplitudes which occur for higher rotational speeds and may ultimately lead to machine failure [2, 6]. As a countermeasure, the compliant and slightly movable foil structure (bump foil and top foil) inside the lubrication gap of a GFB is supposed to dissipate a certain amount of energy via dry sliding friction mechanisms [1, 4], thus reducing the amplitudes of detrimental vibrations [7].

In currently conducted research on GFB rotor systems, sophisticated models and runtime-efficient numerical tools are of major interest with regard to the complexity and costliness of experimental investigations. Considering a fully coupled fluid–structure–rotor interaction model, the gas pressure inside the lubrication gap can be described by a generalized form of the classical Reynolds equation which is applicable for compressible fluids and which yields the bearing forces acting on the rotor journal [3, 5]. Concerning the foil structure, complex FE models as discussed by many recent publications prove to be inapplicable when it comes to a transient analysis of the overall system due to an excessive computational cost. On the other hand, simple elastic Winkler-type foundation models do not capture any frictional effects nor any interaction mechanisms between the bumps. Aiming at accurate results at reasonable computational cost, the minimal dynamic structure model described within this contribution considers energy dissipation assuming a Coulomb-type dry friction law which is applied to a reduced spring–mass arrangement representing the segmented bump foil structure.
The main objective of this study consists in gaining an advanced understanding of the underlying mechanisms leading to beneficial frictional energy dissipation in GFBs. To this end, the nonlinear behavior of the fluid–structure–rotor system is thoroughly investigated by considering stability criteria and by discussing possible bifurcation scenarios with emerging limit cycles. Summing up all results, frictional energy dissipation proves to be of crucial importance with regard to the reduction of undesirable self-excited vibrations.

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S 5 : Nonlinear oscillations

Tuesday 16:30 - 18:30 Marienstr. 7, 2nd floor, Room 206
Chair: Aydin Boyaci (Karlsruher Institut für Technologie)

Comparison of the original and the spectral-system of an elastic rotor in two-lobe bearings with an active geometry adjustment

K. Becker (Karlsruher Institut für Technologie (KIT) - Institut für Technische Mechanik), W. Seemann (Karlsruher Institut für Technologie (KIT) - Institut für Technische Mechanik) 16:30

The improvement of the dynamic behaviour of an elastic rotor supported by journal bearings represents an ongoing field of research, whereby various modifications of the corresponding bearings (compared to the classical cylindrical version) have been proposed in literature.
In order to suppress or at least to decrease unwanted oscillations due to negative effects of instability phenomena of the 'oil-whirl'- and/or 'oil-whip'-type, a two-lobe bearing with an active geometry adjustment is suggested as an alternative approach.
A systematic variation of the bearing's geometry reveals a high potential concerning the stabilization of the rotor at higher rotational speeds.
Nevertheless, this geometry modification of the associated bearings leads to a parametric excitation of the whole system in addition to the already present self-excitation effect ('oil-whirl').
As the modified system tends to very complex behaviour, including quasi-periodic trajectories, a systematic analysis turns out to be very complicated. For investigation reasons the original system is therefore reduced to a Fourier-spectral-system [1].
The basic idea of this reduction is to project the system equations onto a subspace by means of harmonic base functions with the *known* frequency of the parametric excitation [2].
This reduction therefore allows to handle even more complex behaviour like quasi-periodic oscillations by means of the standard methods, involving Eigenvalues and Floquet-multipliers.
A parameter-study, which includes solution continuation algorithms, is carried out, to identify suitable configurations for a reduction of occurring rotor oscillations.
By comparing these results of the spectral systems to those of the original system, a validation of the suggested reduction to a Fourier-spectral-system can be obtained.

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On the numerical approximation of invariant manifolds for quasiperiodic motions

R. Fiedler (University of Kassel), H. Hetzler (University of Kassel) 16:50

In contrast to periodic motions, so far the analysis of quasiperiodic oscillations has not yet become a standard in the vibrational analysis of engineering problems. However, the broad range of self-excited systems subjected to external forcing systematically produces constellations, where oscillations of different physical origin may interfere: in this context, rotor-dynamical problems involving self-excitation and forcing due to unbalance are mentioned as an example of great practical relevance. In general, the presence of different (incommensurable) physical excitation frequencies may lead to quasiperiodic oscillations unless synchronisation occurs.

This contribution aims on a systematic approach to determine stationary quasiperiodic motions by approximating the invariant manifold. Eventually, this approach may be the basis for a continuation of stationary solutions as well as investigations of the stability of such stationary motions. In order to describe a quasiperiodic oscillation an invariant manifold is calculated, whose dimensions are defined by torus coordinates. Therefore it is required that the equations in state-space representation are transformed in amplitudes and phases description. The conventional approach [1] provides a realizable method to calculate invariant manifolds as long as the dimension of the frequency basis is equal to the number of phase angles. Unfortunately, large models of engineering problems often not fulfill this condition and an extension of the standard method is necessary. Within this contribution a partitioning of the phase variables is proposed, which separates torus coordinates from dependent phase angles to overcome this problem. The resulting system of partial differential equations reads

$$\begin{bmatrix} \sum_{k=1}^{p} \dfrac{\partial A_i}{\partial \theta_k} \Omega_k(\mathbf{A}, \boldsymbol{\theta}, \boldsymbol{\varphi}) \\ \sum_{k=1}^{p} \dfrac{\partial \varphi_j}{\partial \theta_k} \Omega_k(\mathbf{A}, \boldsymbol{\theta}, \boldsymbol{\varphi}) \end{bmatrix} = \begin{bmatrix} h_i(\mathbf{A}, \boldsymbol{\theta}, \boldsymbol{\varphi}) \\ \Psi_j(\mathbf{A}, \boldsymbol{\theta}, \boldsymbol{\varphi}) \end{bmatrix}, \qquad \boldsymbol{\theta} \in \mathbb{T}^p, \tag{6.3}$$

where A_i and h_i are the i-th component of the amplitude vector and whose time derivation. Besides φ_j and ψ_j are the j-th component of the vector of dependent phase angles and whose time derivation. Furthermore is $\boldsymbol{\theta}$ the vector of torus coordinates and Ω_k the time derivation of the k-th torus coordinate. The p-dimensional standard torus $\mathbb{T}^p$ is the set which is parametrised over $(0, 2\pi]^p$.

In order to demonstrate the proposed extensions, the method is applied on an unbalanced Laval-Rotor (Jeffcott-Rotor) with linear inner damping and linear and nonlinear outer damping. In this contribution the periodic and quasiperiodic rotor dynamic behaviour is analysed, concerning the dimension of the invariant manifold. Simulations show that the stability limit of periodic orbits change, if the eccentricity of the center of mass is varied. An extended area of periodic oscillations is the result. Furthermore, the method allows a tracing of a quasiperiodic solution regardless of the stability. To identify the latter a criterion to assess the stability of solutions on an invariant manifold is investigated [2].

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Non-linear vibration localisation through modulation instability in cyclic and symmetric structures

F. Fontanela, A. Grolet, L. Salles, A. Chabchoub, N. Hoffmann (Imperial College London) 17:10

Localisation of vibrations in aerospace structures has been widely studied in the last three decades. In the linear regime, localised vibrations arise due to inhomogeneities resulting from manufacturing processes, and engineers usually refer to this phenomenon as mistuning. More recently, attention has also been given to vibration localisation due to non-linear effects, where localised solutions can arise even in perfectly symmetric structures through bifurcations. Moreover, it is well accepted in the vibration engineering community that travelling wave states can emerge in rotating machines, e. g. due to aeroelastic excitation and Coriolis effects. Therefore, this research investigates the effects of travelling waves and their corresponding non-linear evolution through envelope dynamics. The results show spatio-temporal localisation when travelling waves are excited in their unstable regime.

Oscillations of a visco-elastic belt drive

A. Steindl (TU Wien) 17:30

We investigate the loss of stability of the steady configuration of a planar visco-elastic belt drive. The belt is considered as a linearly visco-elastic slender beam with small bending stiffness, which is driven by a steadily rotating drum. Due to the presence of the small damping parameter and the small bending stiffness, the equations of motion are severly singularly perturbed.
By variation of system parameters, like the driving speed, the damping coefficient, the tension force and the radius of the drums, we calculate the steady configuration and the stability limit of the belt. Preliminary calculations indicate, that the viscous damping and the strong bending at the drums can decrease the critical driving speed significantly and lead to flutter oscillations.

A Simple Approach of Contact Acoustic Nonlinearity (CAN) for the Scaled Boundary Finite Element Method (SBFEM)

J. Bulling (BAM Federal Institute for Materials Research and), J. Prager (BAM Federal Institute for Materials Research and Testing) 17:50

In modern non-destructive evaluation and structural health monitoring applications guided ultrasonic waves are used to identify flaws such as cracks. Particularly cracks can lead to a nonlinear response if a propagating wave passes. At least for higher defections

the propagating wave excites each side of the crack in such way that it hits the other side. This clapping generally leads to a generation of higher harmonic waves. To get a better insight into the salient physics of the effect numerical simulations are necessary.
In the recent years, the Scaled Boundary Finite Element Method (SBFEM) was introduced to efficiently simulate guided wave propagation in plates and shells. The main advantage of the method is that it needs only a discretization of the boundary instead of the whole domain. This leads to an easy modeling of cracks and especially of the crack tip. The SBFEM approach is still related to the Finite Element Method and uses similar techniques. The method is very efficient using high-order-spectral elements.
In this contribution, we present a short introduction into the basics of SBFEM formulation of the dynamic elastic wave equation. The SBFEM is then extended for modeling the non-linear behavior of crack clapping. Different approaches with increasing complexity are presented and assessed with respect to numerical stability.
Keywords. Ultrasound, Guided Waves, Numerical Simulation, Scaled Boundary Finite Element Method, Contact Acoustic Nonlinearity

S 5 : Nonlinear oscillations

Thursday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 105
Chair: Dominik Kern (TU Chemnitz)

Structural stability of nonlinear valve train systems in automotive engines

M. Busch (Schaeffler Technologies AG & Co. KG) 16:30

Valve train systems are applied in automotive combustion engines to accomplish the alternation of load. With a rotating cam, a roller-finger follower is pivoted which, in turn, moves a valve shaft vertically within its guide. If the valve opens, i.e., if the valve shaft detaches from its seat, the fresh fuel-air mixture is fed into the cylinder or the exhaust gas of finished combustion process is ejected from the cylinder.
In the presentation the structural stability of a valve train system is investigated. A stable operation of the system is crucial for the efficiency of the engine. Further, the stability behavior is important from a simulation point of view since instabilities are challenging for numerical solvers.
Depending on the rotation direction of the cam, the valve train system can be applied in a pushed and in a pulled design version. From test-rig measurements it is known that pushed valve trains can suffer from higher oscillation and larger friction. In the presentation it is shown that pushed valve trains entail a structural instability, i.e., the roller-finger follower runs close to an unstable equilibrium while in pulled valve trains the equilibrium is stable.
Due to the clearances in the valve train, the roller-finger follower performs a three-dimensional rotary motion with a periodically oscillating center of mass. For higher cam speeds, a subcritical pitchfork bifurcation occurs and the unstable valve train stabilizes

itself. This velocity-dependent stabilization effect was also investigated for inverted pendulums with vibrating suspension, see the work of Pjotr Kapitza from 1951.
For analyzing the system, a simplified pendulum replacement model is derived. The stability analysis is carried out in an analytical manner by investigating the effective potential energy of the model. The stability results are validated with a transient simulation using a numerical time integration.

Self-excited oscillations of calendering units due to time delay

A. Boyaci (Karlsruher Institut für Technologie), W. Seemann (Karlsruher Institut für Technologie (KIT) - Institut für Technische Mechanik), E. Keskinen 16:50

In manufacturing of paper, thin foils and metal sheets, two cylindrical rolls are in rolling contact through which a web-like thin material is passed in order to further smooth and form it. In paper machines, one of the rolls is covered by a polymer layer to provide a wider contact zone which allows higher rotational speeds due to the longer web manipulation time. However, with increasing rotational speeds, the regenerative effect of the viscoelastic cover polymer leads to time-delay instabilities of the rolling contact system which result in self-excited oscillations [2, 3, 4, 5, 6].
In this contribution, the mechanical model of a two-roll system is considered where the viscoelastic properties of the cover are accounted by a rheological model in the contact zone. Hence, the linearized equations of motion can be stated as a system of delay differential equations. To determine the critical delays and speeds, respectively, stability analyses are carried out by applying matrix pencil methods [1]. Thus, the original eigenvalue problem, which is represented by a quasi-polynomial, is splitted into two different linear eigenvalue problems. Then, the obtained stability charts illustrate the critical rotational speeds against different design parameters and show the typical wave-like roll cover deformation patterns of various order numbers.

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Influence of Ultrasound on Friction-Induced Vibrations during Tightening of Bolted Joints

N. Baramsky (Hamburg University of Technology), A. Seibel (Hamburg University of Technology), J. Schlattmann (Hamburg University of Technology) 17:10

In the last few years, a lot of work including analyses on screw-threaded fasteners had been done. Methods had been developed and technical rules had been set up, which focused on the quality of the industrial screw assembly. But users of partly and fully automated screwdriver systems still have to deal with failures during the tightening process. One reason for these failures are rotational vibrations. As practice has shown, these rotational vibrations are strongly influenced by special underhead geometries, certain material pairings, the screw-in depth, the screwdriver speed, and the usage of socket wrench extensions. The vibrations are primarily friction-induced and can lead to an inaccurate measurement of the tightening torque and thus to an improper clamping force. This, in turn, can lead to assembly errors resulting in tool damage or screw failures.

For this reason, a multibody model was presented in (Baramsky et al., 2015) which can reproduce the rotational vibrations during the tightening process. In this publication, we study the influence of ultrasonic vibrations induced by a transducer. In particular, we investigate the effects of ultrasound on the stick-slip behavior. Consider a bolted joint connection, which is represented by a multibody model with three degrees of freedom, where the bearing, the shaft, and the thread part of the screw can move about their rotational axis. The joint is tightened by implying a torque at the bearing. In addition to that, a rotational sinusoidal torque is implied at the head of the screw. The frequency and magnitude of the latter torque is varied to investigate the influence on the overall dynamic behavior. Based on the knowledge of the multibody system, a set of frequencies can be identified that will excite the system in resonance to different eigenfrequencies thus decrease the effect of stick-slip during the tightening process.

The stick-slip behavior reduces the continuous application of clamping force to a more discrete form since the system only comes to rest at the stick phase of the vibration. Decreasing the magnitude of these steps leads to a more precise control of the pretension force. Advanced knowledge on the reaction of the multibody system on ultrasonic vibrations enables the industry to develop highly optimized tightening mechanics to further improve the reliability of bolted joint connections.

Baramsky, N.; Seibel, A.; Schlattmann, J.: Modeling of Friction-Induced Vibrations during Tightening of Bolted Joints. In: Proceedings in Applied Mathematics and Mechanics, 16:259-260, 2015.

A note on a double-serial switch-spring-parallel semi-active connection element

M. Dahlmann (TU Ilmenau), C. Min, T. Sattel 17:30

Subject is a semi-active connection element consisting of two identical subsystems in series. Each subsystem is composed of one spring and one switch in parallel. The switch can prevent spring movement when closed. Thus, the potential energy in the spring is stored. Other authors often disconnect the spring so that the energy is dissipated. The use of two subsystems in series allows to direct power from extension and compression into different springs. Therefore, one switch is open and the other is closed simultaneously, yielding two states which allow to control the force exerted on a connected mass. The averaging method and the mass inertia allow to control the positions of a connected mass. Thus, the semi-active connection element behaves similar to an actuator with the limitation that the average work vanishes. Averaging is applicable for a position where chattering with the high switching frequency is neglected. The force remains highly discontinuous. Possible applications are vibration reduction at low frequency, shock absorption into potential energy of the springs, or control of equilibrium positions.

Considering Nonlinearities to Design Micro System's Vibrational Sensitivity

D. Roeser, S. Gutschmidt, T. Sattel 17:50

In contrast to macro scale mechatronic system, the nonlinear effects present in micro electro mechanical systems (MEMS) cannot be neglected. Some applications like scanning probe microscopy (SPM) are based on nonlinear interaction forces between probe and sample to image its topography. Despite these nonlinearities, the design of MEMS is mainly based on a linear methodology. Recently, considering nonlinear behavior in the design process to increase the performance metrics of MEMS has drawn more attention. In this work, the impact of nonlinearities on the sensitivity of MEMS sensors measuring quantities based on a change in resonance frequency is analyzed. In this case, the sensor is an array of cantilevers which are individually actuated by means of Joule heating and have an integrated piezoresistive displacement sensor as well as a composite structure and varying cross section. The mathematical model is based on a coupled thermoelastic equation of motion which has a direct and a parametric excitation. Latter leads to an excitation of integer multiple of the excitation frequency. Nonlinearities considered result from a nonlinear potential with a quadratic and cubic stiffness. These nonlinearities originate from a tip sample interaction (e.g. SPM) and a nonlinearity introduced by design (e.g. by control or structural change to utilize a prestress).
The results show the influence of internal/parametric resonances as well as a hardening/softening nonlinearity on the amplitude and phase change per change in measured quantity (e.g. tip-sample distance, mass of a particles). Conclusions are drawn on the utilization of such effects to increase the performance metrics of the sensor. For instance by using a saturation effect based on an internal resonance to increase the amplitude response to a change in measured quantity.

S 6: Material modelling in solid mechanics

Organizers: Michael Johlitz (Institute of Mechanics, Universität der Bundeswehr München)
Alexander Lion (Universität der Bundeswehr München)

S 6a : Material modelling in solid mechanics

Tuesday 14:00 - 16:00 Marienstr. 13, 1st floor, Lecture hall B
Chair: Alexander Lion (Universität der Bundeswehr München)

On the modeling of a transient creep using a nested multiplicative split of the deformation gradient

A. Shutov (Lavrentyev Institute of Hydrodynamics), A. Larichkin (Lavrentyev Institute of Hydrodynamics), V. Shutov (Novosibirsk State University of Architecture, Design and Arts) 14:00

A new phenomenological model of cyclic creep is proposed which is suitable for applications involving finite creep deformations of the material. The model accounts for the effect of the transient increase of the creep strain rate upon the load reversal. In order to extend the applicability range of the model, the creep process is fully coupled to the classical Kachanov-Rabonov damage evolution. As a result, the proposed model describes all the three stages of creep. Large strain kinematics is captured in a geometrically exact manner using the assumption of a nested multiplicative split, originally proposed by Lion for finite strain plasticity. It is shown that the model is thermodynamically admissible, objective, and w-invariant. Implicit time integration of the proposed evolution equations is discussed. The corresponding numerical algorithm is implemented into the commercial FEM code MSC.MARC. The model is validated using this code; the validation is based on real experimental data on cyclic torsion of a thick-walled tubular specimen made of the D16T aluminium alloy. The numerically computed stress distribution exhibits a "skeletal point" within the specimen, which simplifies the analysis of the test data. The generalization of the advocated approach to the analysis of creep-plasticity interaction is also discussed.

A large-strain phase-field model for nematic elastomers based on Landau-de-Gennes theory

M. Keip (University of Stuttgart), O. Nadgir (University of Stuttgart) 14:20

Liquid-crystalline elastomers (LCE) are some of the most fascinating materials of our time. They combine the properties of rubber and the properties of liquid crystals and thus show extraordinary effects [1, 2]. For example, they react mechanically to a number of physical fields, such as electric and magnetic fields, temperature, and light. When exposed to those fields, they experience very large mechanical deformations and can therefore be used in innovative technical applications [3]. A particular type

of liquid crystal elastomers is given by nematic LCEs, which show a phase transition between an isotropic and an anisotropic (nematic) state. In the present talk, we derive a phase-field continuum model for nematic LCEs based on Landau-de Gennes theory [1]. A symmetric and traceless tensorial order parameter is used to mimic the fundamental characteristics of the nematic behaviour [4]. Furthermore, neo-classical Warner-Terentjev elastic energies [5] are employed to account for the inherent finite nemato-elastic deformations. Representative numerical simulations will highlight the underlying material characteristics such as nemato-mechanical domain evolution, defect annihilation and stripe-domains formation under different types of boundary conditions.

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Third-order elastoplasticity and thermoplasticity

J. Reiher (Otto-von-Guericke-Universität), A. Bertram (Otto-von-Guericke Universität Magdeburg) 14:40

Assuming the existence of an observer-independent power functional, a constitutive framework for a general third gradient elasticity for finite deformations is suggested by extending the concepts in [Bertram 2014] and [Bertram 2015]. Material variables are introduced that allow to measure generalized strain and stress in a third-order material. These variables are derived from the principle of virtual power. From the transformation behavior of these variables under changes of the reference placement a generalization of the concept of elastic isomorphy is derived. This concept allows to define what it means that two third-order materials have the same elastic behavior. A generalization of the concept of material symmetry and symmetry groups for third-order materials is presented. Building upon the results in elasticity a framework for third-order plasticity is established which relies on the assumption that all elastic ranges of a material during a plastic deformation process are isomorphic. The concepts of yield criteria as well as of flow and hardening rules are generalized for the third-order case, and the plastic dissipation is calculated. Finally it is shown that third-order materials can be modeled in a thermodynamically consistent form. This is done by introducing

the set thermodynamic variables that account for the first and second gradient of the strain and the Helmholtz free energy. The elastic and plastic behavior of a third-order material, is then embedded into the thermodynamical framework. The second law of thermodynamics in the form of the Clausius-Duhem inequality yields the thermoplastic potential for the generalized stresses as well as restrictions of the yield and hardening rules. It is also shown how elastic and plastic deformations contribute to changes of the temperature.

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Grain boundaries kinetic in poly crystalline material using orientation dependent interface energy.

A. Khan (Ruhr Universität Bochum/ Lehrstuhl für Mechanik - Materialtheorie), K. Hackl (Ruhr Universität Bochum), M. Baitsch (Ruhr-Universität Bochum) 15:00

The Polycrystalline materials grain boundary structure, crystalline texture and grain surface morphology, each plays an important role in interface transport. Among the different surface evolution method, the object of current work is to study the kinetics of interfaces by diffusion only. Most of the existing theoretical and computational models, used two dimensional grooving with one dimensional surface evolution. Hackl et al [1] has presented novel variational model of interface motion using thermodynamic extremum principle for grooving and wetting under diffusion. This model is further extended to 3D using 2D surface evolution. A coupled motion of an interface in polycrystalline material with symmetric boundaries is studied. Since, most of the polycrystalline material are non-symmetric and periodic in nature. In this paper, kinetics of periodic polycrystalline aggregate is studied. An ansatz function for grain boundary energy is defined as a functional of grain orientation and boundary inclination. For such orientation dependent grain boundary energy, Herring's relation must be satisfied locally at each triple line thus we have a four set of equations at each triple line in Periodic RVE. Such an over determine system is solved using non-linear optimization method with weak constraint for interface energies. In these simulations, surface mobility is considered to be constant in all directions. A comparison between orientation dependent evolution with other model is done.

A slip gradient crystal plasticity theory based on an extended energy flux

A. Prahs (Karlsruhe Institute of Technology (KIT)), T. Böhlke (Karlsruhe Institute of Technology (KIT)) 15:20

Microstructured materials exhibit a non-local mechanical behavior, such as the Hall-Petch effect, that has been experimentally investigated for several metals, e.g., [1]. The behavior of, e.g., oligo- or polycrystals is influenced by the presence of grain boundaries (GB) constituting a resistance against the dislocation movement. Such a non-local mechanical behavior cannot be reproduced by classical plasticity theories due to the lack of an internal length scale. Gradient plasticity theories, which are ranged in the class of extended continuum models, overcome this drawback, introducing the internal length scale, e.g., by means of an defect energy, e.g., [2]. The work at hand discusses, how extended continuum models, e.g., [3], can be related to an enhancement of a dislocation based energy flux, in general. This is illustrated by the derivation of a slip gradient crystal plasticity theory regarding small deformations. The presented theory accounts for the crystallographic orientation of adjacent grains using a free energy for the grain boundary proposed by [4]. Moreover, an analytical, one dimensional solution, with respect to single slip, for a homogeneous stress state is discussed.

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[3] S. Forest, Micromorphic approach for gradient elasticity, viscoplasticity, and damage, J. Eng. Mech. 135, 117-131 (2009)

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A multisurface model for gradient-enhanced damage coupled to finite plasticity

L. Sprave (Institute of Mechanics, TU Dortmund), A. Menzel (Institute of Mechanics, TU Dortmund and Division of Solid Mechanics, Lund University) 15:40

A gradient-enhanced damage formulation is coupled to isotropic plasticity in the framework of finite strains. Within the finite element method an additional field variable, representing nonlocal damage, is introduced and linked to its local counterpart to allow a standard local formulation at the material point level. The onset of damage and plasticity is governed by damage and yield criteria respectively. This multisurface approach requires the determination of the two Lagrange multipliers. Utilising logarithmic strains, a formulation in principal axes in combination with a von Mises yield criterion is

implemented. The damage functions are defined by means of exponential functions in order to avoid further constraints on the local damage variable. The model is able to capture a wide range of material responses, ranging from brittle to ductile damage and plasticitiy dominated behaviour. The mesh independence of the model is shown by means of representative finite element examples.

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2. B. Kiefer, T. Waffenschmidt, A. Menzel and L. Sprave, A gradient-enhanced damage model coupled to plasticity - multi-surface formulation and algorithmic concepts, International Journal of Damage Mechanics, accepted for publication (2016)
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4. T. Waffenschmidt, C. Polindara, A. Menzel and S. Blanco, A gradient-enhanced large-deformation continuum damage model for fibre-reinforced materials, Computer Methods in Applied Mechanics and Engineering, vol 268, p. 801-842 (2014)

S 6a : Material modelling in solid mechanics

Tuesday 16:30 - 18:30 Marienstr. 13, 1st floor, Lecture hall B

Chair: Sahir Butt (Ruhr-Universität Bochum)
Carla Beckmann (Fraunhofer-Institut f.Werkstoffmechanik IWM Freiburg)

Wave dispersion and propagation is a linear peridynamic solid

S. Butt (Ruhr Universität Bochum), G. Meschke (Ruhr Universität Bochum) 16:30

Peridynamics is a nonlocal continuum model which offers benefits over classical continuum models when there are discontinuities present in the deformation. However, the nonlocal characteristics of peridynamics lead to a dispersive dynamic response of the medium. In this study we focus on the dispersion properties of a state-based linearized LPS model and specifically investigate the role of the peridynamic horizon. We derive the dispersion relation for one, two and three dimensional cases and investigate the effect of horizon size and mesh size, as well as, of the influence function on it. For validation, the dispersion curves obtained from peridynamics are compared with experimental data for two kinds of sandstone. It is also shown that the dispersion modeling done in the

proposed way is mesh independent. Finally, we show how the influence function can be used to minimize wave dispersion and demonstrate it qualitatively by wave propagation in one and two dimensional peridynamic medium.

Mechanically coupled phase field based simulation of the solid-electrolyte interface growth in lithium ion battery

Y. Bai (TU-Darmstadt), B. Xu 16:50

Lithium ion batteries have been widely applied in our daily life. For this battery, the chemical reaction between anode and electrolyte will form a solid electrolyte interface (SEI) layer. The SEI layer formed on the anode surface is irreversible and it will consumes lithium ions and lead to the capacity fade, so it plays an important role for the battery life and performance [1]. Different mathematical models have been developed to describe the growth of SEI layer [2-6]. Phase-field models have emerged as an elegant method to track the evolving interface between the electrolyte and the anode material [7]. However, its impact on the stress distribution and the deformation behavior of the bulk electrode has not been investigated yet in the literature. In fact, the SEI acts as an additional constraining layer on the electrode surface, and it induces fracturing during the cycling. In this study, we describe a model for the evolution of the SEI on electrode particles, together with its interactions with the mechanical behavior of the solid. The model is based on the work of Guyer [7], Bazant [8] and Stein [9], with the order parameter describing the transition between liquid electrolyte and solid electrode. We describe the model and its implementation and use some benchmarks to study the stress distribution inside the SEI phase during the SEI growth.

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On the Modelling of Memristive Material Behavior in the Context of the Finite Element Method

J. Obst (Institute of Mechanics and Shell Structures, TU Dresden), A. Franze (Institute of Mechanics and Shell Structures, TU Dresden), D. Balzani (Dresden Center for Computational Materials Science (DCMS)) 17:10

In 1971 Leon Chua came up with an idea for a device that 45 years later is on the verge of revolutionizing electronics (cf. [1]). For reasons of symmetry he argued that this electric device completes the basic electric circuit with resistor, capacitor and inductor. The device he postulated is called memristor. This word is a portmanteau of memory and

resistor and describes an element whose properties depend on the history of the input function and which maintains its inner state if no external excitation is present. Out of these properties, Chua predicted a memory effect for the memristor, which seems currently to be the main application of this device in the field of electrical engineering. As analogies have a long tradition in various fields of science it is quite obvious to transfer these ideas from electric circuit theory to mechanics by electro-mechanical analogies. This transfer already led to a generalized classification of devices for dynamical systems [2]. In particular a mechanical memristor for a system with one single degree of freedom is a displacement-dependent dashpot.
To investigate the behavior of continuous solids which show memristive properties, the development of suitable three-dimensional material models is aimed. Thus, this paper investigates the implementation of a memristive material model in the context of the Finite Element Method. Therefore, one-dimensional memristive material models are analyzed and a continuum-mechanical, memristive material model is developed based on a Kelvin-Voigt-Model. Multiple example problems are simulated to verify the characteristics of this particular material class. In Particular, the slipknot-shaped hysteresis of the stress-strainrate-curve and the typical behavior for increasing excitation frequencies can be shown.

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Computational generation and computational homogenization of open porous asphalt structures based on XRCT scans

D. Wingender (Institute for Computational Engineering, Ruhr-Universität Bochum), R. Jänicke (Department of Applied Mechanics, Chalmers University of Technology) 17:30

X-ray Computed Tomography (XRCT) scans show that open porous asphalt is a complex structure containing three different phases: elastic mineral aggregates, a visco-elastic bitumous binder and voids. To computationally investigate the overall material behavior of this structure, we generate a representative volume element (RVE) of the geometrical structure of asphalt concrete. To reproduce this structure, XRCT scans could be used, but a high computational expense to get the geometry occurs due to the richness of topological information of these scans. To avoid this, we extract microstructural parameters to generate artificial and simplified asphalt concrete structures.
In the present contribution, these parameters are the volume fractions of the three phases and the particle size distribution of the aggregates. Based on these, the asphalt concrete structure can be generated computationally. Therefore the weighted Voronoi tessalation is applied on spheric particles with predefined sizes, that are contributed by a discrete element simulation via the Lubachevsky-Stillinger algorithm in a periodic cube [1]. After shrinking the Voronoi cells statistically, the newly formed cells represent the

mineral aggregate while the rest of the cube is assumed to contain the bitumous agent and voids. Since, for practical applications, the chosen volume elements are far from being truely representative, we call them Statistical Volume Elements (SVE).
The main focus of this work lies on the spatial allocation of the bitumen and its computational generation within the space between the concrete particles. This generated three phase structure is homogenized by simulating creep and relaxation tests to investigate the overall material response using material data from experiments with pure bitum.

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Numerical solution of plane constrained shear problem for single crystals within continuum dislocation theory

T. Tran (Lehrstuhl für Mechanik-Materialtheorie, Ruhr Universität Bochum, D-44801 Bochum, Germany), M. Baitsch (Bauinformatik und Numerische Verfahren, Hochschule Bochum, D-44801 Bochum, Germany), K. Le (Ruhr Universität Bochum) 17:50

Within the recently proposed Continuum Dislocation Theory (CDT), numerical solutions of simple shear test for single crystals strip using finite elements are performed. Under the assumption of plane constrained deformation of crystal having only one active slip system, the plastic slip, the dislocation density as well as the stress-strain curve are computed. The results of numerical simulations are compared with those obtained from analytical solutions which show good agreement.

A probabilistic analysis to identify a correlation between cell characteristics and the effective material properties in solid foams

C. Beckmann (Fraunhofer-Institut für Werkstoffmechanik IWM), J. Hohe (Fraunhofer-Institut für Werkstoffmechanik IWM) 18:10

Materials with a heterogenous microstructure, as solid foams, always implicates a scatter in the macroscopic effective material properties. To consider these material uncertainties in the design of components with micro heterogeneous parts, a probabilistic analysis of the most important microstructure properties is of greatest use. In the present study, the influence of the local cell density as well as the cell size and orientation on the macroscopic effective material properties is analyzed. For this purpose, statistical representative finite element models are generated to determine a correlation between the stiffness components of each cell and its geometric characteristics. Afterwards, on the base of this assessment a probabilistic computational procedure is derived. This is a big benefit, because it allows to predict the material scatter in cellular materials without generation of complex finite element models representing the real geometry of the microstructure. Instead of such time-consuming computations a random field discretization is applied. Therefore, the random field variables describe in terms of probabilistic distributions

the most essential influence of the local microstructure properties on the macroscopic effective material properties.

S 6a : Material modelling in solid mechanics

Wednesday 14:00 - 16:00 Marienstr. 13, 1st floor, Lecture hall B
Chair: Hans Wulf (TU Chemnitz)
Chris Leistner (TU Clausthal)

Multiscale Modeling of Strain-Induced Crystallization in Polymers

S. Aygün (Institute of Mechanics, TU Dortmund University, Germany), 14:00
S. Klinge (Institute of Mechanics, TU Dortmund University, Germany),
J. Mosler (Institute of Mechanics, TU Dortmund University, Germany),
S. Govindjee (University of California, Berkeley, USA)

The strain-induced crystallization (SIC) in polymers is a phenomenon manifesting itself as the natural reinforcement caused by the high deformation or by the reduction of the temperature. It is typical for natural rubber, since this material contains more regularly oriented chains than the other polymers. It has been evidenced that SIC occurs instantaneously after deforming the material to sufficiently high stretches. In natural rubber, the crystallization starts at a strain of 200-400%, whereas maximal possible strains amount up to 700%. Most of the models focusing on the modeling of polymers use the Langevin expression for the free energy as a basis [1, 2]. The current presentation, however, treats a polymer affected by the strain induced crystallization as a heterogeneous medium consisting of regions with a different degree of network regularity. Such a concept allows the depiction of the nucleation and the growth of crystalline regions as well as the change of effective material parameters depending on the level of the strain applied. The model proposed is thermodynamically consistent. It is based on the assumptions for the free Helmholtz energy and dissipation potential. Both of them primarily include bulk terms due to the deformation and crystallization. The external variable is the deformation, whereas the inelastic deformations and degree of the network regularity are internal variables. Their evolution equations are derived according to the principle of miniumum of dissipation potential [3]. The explained framework is advantageous for several reasons. First, it is suitable to answer the crucial question as to which process predominantly influences SIC: the nucleation of new crystalline regions or the growth of already existing ones. Secondly, the proposed model is ideal for a direct implementation within the standard multiscale finite element concept [5]. This numerical homogenization procedure is compatible with the theory of finite strains and is applicable for modeling those cases where the ratio of characteristic lengths of scales tends to zero. Both of these features are necessary for the effective modeling of SIC.

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Determination of the elastic behaviour of hybrid-yarn reinforced elastomers using twisted-periodic boundary conditions

J. Storm, M. Kaliske (TU Dresden) 14:20

Reinforcements of elastomers using hybrid-yarns allow to take advantage of the bi-modular stiffness behaviour of those yarns.The initial deformation behaviour is characterised by low stiffness and the potential for finite deformations. Reaching a specifc limit of hybrid-yarn stretch, the mechanical behaviour changes towards larger stiffness and only allows for small further deformations. In comparison to other yarn reinforcements with finite deformations the achieved material strength is relatively high.To obtain the macroscopic elastic constitutive equations, the talk firstly considers the geometry and the initial eigenstress configuration of the meso-scale.The bending behaviour of the involved yarns is approximated using anisotropic hyperelastic material laws.The effciency of the applied computational homogenisation method is significantly improved by introducing twisted-periodic boundary conditions.On macro-scale a hyperelastic approach for elastomers is extended by ananisoptropic term representing the yarn reinforcement.

An Affine Micro-Sphere Model for Strain-Induced Crystallization in Rubbery Polymers

A. Nateghi (University of Stuttgart), M. Keip (University of Stuttgart), C. Miehe (University of Stuttgart) 14:40

Upon stretching a natural rubber sample, polymer chains orient themselves in the direction of the applied load and form crystalline regions. If the sample is retracted, the original amorphous state of the network is restored. Due to crystallization, properties of rubber are considerably altered. The reinforcing effect of the crystallites leads to stiffening of the rubber and an increase in the crack growth resistance. Hence, it is of great importance to understand the mechanism leading to strain-induced crystallization. However, limited theoretical work has been done on investigation of the kinetics of strain-induced crystallization.

Strain-induced crystallization in natural rubber has been extensively studied using *X-ray diffraction* technique. Recent developments in this technique have made it possible to evaluate the instantaneous crystalline mass fraction during loading and unloading of the rubber specimen. A key characteristic observed in the stress-strain diagram of

strain crystallizing rubber is the development of a hysteresis. This hysteresis is entirely attributed to strain-induced crystallization.
In this work we propose a micro-mechanically motivated material model for strain-induced crystallization in rubbers. Our point of departure is constructing a micro-mechanical model for a single crystallizing polymer chain. Subsequently, a *thermodynamically consistent* evolution law describing the kinetics of crystallization in the chain level is proposed. This chain model is then incorporated into the *affine micro-sphere model*. Microscopic free energies of individual semi-crystalline polymer chains are homogenized over the three-dimensional orientation space to obtain the macroscopic free energy of the rubbery material. Finally, the model is numerically implemented and its performance is compared with the experimental data.

[1] C. Miehe, S. Göktepe and F. Lulei. 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* 52 (2004), 2617–2660.

[2] S. J. Mistry and S. Govindjee, A micro-mechanically based continuum model for strain-induced crystallization in natural rubber. *International Journal of Solids and Structures* 51 (2014), 530–539.

[3] M. Kroon, A constitutive model for strain-crystallising Rubber-like materials. *Mechanics of Materials* 42 (2010), 873–885.

[4] J. Guilie, L. Thien-Nga and P. Le Tallec, Micro-sphere model for strain-induced crystallization and three-dimensional applications. *Journal of the Mechanics and Physics of Solids* (2015).

Experimental investigation and modelling of volume shrinkage in curing epoxy resins

C. Leistner (Clausthal University of Technology), J. Wittrock (Clausthal University of Technology), D. Abliz (Clausthal University of Technology), G. Ziegmann (Clausthal University of Technology), S. Hartmann (Clausthal University of Technology) 15:00

Fiber composite materials offer many advantages in lightweight construction. They combine at least two components, fibers and a matrix material. Epoxy resins are widely used as matrix material. During production process, these epoxy resins cure by an exothermic chemical reaction. Due to low thermal conductivity, heat can hardly be transported, which results in an inhomogeneous temperature distribution and a further influence on the curing process. Especially for thick walled structures, one can observe warpage or cracks inside the final components. Even combustion might occur during curing. The cracks are a result of residual stresses, which develop because of chemically shrinking material.

In this presentation, the properties of a pure hot curing epoxy system has been investigated. The curing kinetics can be found by a set of DSC measurements that is one way to determine a degree of cure. There do not exist established methods for determining the shrinkage. To this end, shrinkage measurements based on Archimedes' principle are carried out for pure epoxy resin at different curing temperatures. These results can be correlated with the curing kinetics.
The curing model combines a reaction approach of n-th order and a term that reflects the diffusion control. The shrinkage is a volumetric chemical part of the strain, which depends on the degree of cure. The whole experimental process is explained and the resulting model calibration will be shown.

Thermomechanics of strain-induced crystallization in carbon black filled natural rubber under cyclic loading

L. Zybell (Leibniz-Institut für Polymerforschung Dresden e.V.), J. Domurath (Leibniz-Institut für Polymerforschung Dresden e.V.), K. Schneider 15:20

Strain-induced crystallization in natural rubber has been widely investigated in the last decades by different scattering techniques. Due to dissipative processes and structural changes in the material, deformation processes are accompanied with a significant amount of heat production. Time-resolved wide-angle X-ray diffraction (WAXD) was used to characterize the structural changes in the material and the local degree of crystallinity during mechanical deformation. By the simultaneous use of an infrared thermography system, the scattering results could be combined with changes in the internal energy due to dissipation and crystallization resp. melting of the crystallites.
A thermal model which includes the heat exchange to the environment enables the separation of the different heat sources. It can be applied to quasi-static as well as cyclic loading to different strain levels and improves the understanding of the processes of structural changes and the temperature and structure dependent mechanical properties of rubber materials. Finally, the effect of different amount of carbon black filler on the evolution of crystallinity and the corresponding thermomechanical response of natural rubber under cyclic loading is discussed.

Simulation of self-organization processes in filled rubber

H. Wulf (Chemnitz University of Technology), J. Ihlemann (Chemnitz University of Technology) 15:40

During experimental characterization of filled rubber specimen, prestraining leads to a reduction of the stress response at smaller strain values, known as Mullins effect (Mullins 1948). Hereby, an anisotropy is induced, as the softening relates to the direction of the prestrain. When the material is loaded in a lateral direction afterwards, a continued softening can be observed (Besdo et. al. 2003). The work intends to examine the physical reasons for this material behavior, which are still subject of discussion.
This contribution is based on a theory developed by Ihlemann (Ihlemann 2003), which explains the Mullins effect as a result of self-organization processes based on weak

physical bonds. The main idea states that the physical bonds organize into a pattern consisting of areas with high and low linkage densities. The theory is investigated by a simulation program using an abstract meso-scale model of the molecular structure of filled rubber. All interactions are modeled by simple elastic elements. Nevertheless, the model shows a variety of complex nonlinear properties. Typical rubber behavior, like Mullins effect is successfully reproduced. Moreover, within the model a self-organization process can be clearly observed. Hence, the simulation provides strong evidence for the relevance of self-organization for rubber behavior.

Mullins, L. 1948: Effect of stretching on the properties of rubber. Rubber Chem. Tech. 21, pp. 281-300.

Besdo, D., Ihlemann, J., Kingston, J.G.R. and Muhr, A.H. 2003: Modelling inelastic stress-strain phenomena and a scheme for efficient experimental characterization. In: Busfield, J.J.C. and Muhr, A.H. (eds): Constitutive models for rubber III: 309-317. Lisse: Swets & Zeitlinger.

Ihlemann, J. 2003: Kontinuumsmechanische Nachbildung hochbelasteter technischer Gummiwerkstoffe. Düsseldorf: VDI-Verlag.

S 6b : Material modelling in solid mechanics

Wednesday 14:00 - 16:00 Marienstr. 13, 1st floor, Lecture hall D

Chair: Stefan Hartmann (TU Clausthal)
Eray Arslan (Inonu University)

Determination of Material Parameters from Imperfect Cyclic Plasticity Test Data

E. Arslan (Inonu University), W. Mack (TU Wien), M. Zigo (MAGNA STEYR Engineering), G. Kepplinger (MAGNA STEYR Engineering) 14:00

The investigation of the ultra low cycle fatigue behavior of engineering structures in the automotive industry [1] requires the determination of material parameters in the elastic-plastic range, particularly with respect to hardening. After a suitable hardening model for the material under consideration has been chosen, the model parameters must be fitted to the corresponding (uniaxial) cyclic tension-compression test data, which are usually the only ones available from standard test devices. In literature, several procedures for fitting the material parameters for different types of material models and load cycles during the tests were proposed [2], [3].
In general, a combined nonlinear isotropic-kinematic hardening model is the most suitable one for implementation in an FE-model of a structure subject to cyclic loading [2], [5]. The test data for its parametrization are obtained from cyclic strain controlled

tests in specified strain ranges [5]; e.g., a multi-step method may be applied, where a specimen is cycled at constant strain amplitude until the material behavior has stabilized, and then there follows another block of loading cycles with higher strain amplitude until re-stabilization, and so on. Since the material parameters thus determined then are used in the FE-models for nonlinear FEM simulation and later on for fatigue life analysis, reliability of material data and the results based thereon is essential for the sustainability of the further design process. However, the cyclic tension-compression test data may exhibit some problematic features. For instance, loading and unloading parts in the elastic region may not have exactly the same slope (as should theoretically be the case), or the hysteresis curve may not have sharp corners which are necessary to determine the hardening parameters. Moreover, the strain data provided by the test device may a little bit exceed the limits even though a certain strain range was prescribed. Some reasons of these inaccuracies of the test data may be an inappropriate strain rate during loading or not very high sensibility of the measuring and/or loading tools of the test device. Although in general each of the errors individually is small, they may all in all nevertheless create considerable uncertainties of the material parameter values.
Hence, whereas the hitherto in literature given procedures for the determination of the material parameters generally are based on "perfect" test data, this contribution is devoted to answering the question how to calculate them reliably from "imperfect" data. Specifically, the issues of apparently different elastic behavior during loading and unloading phases, scattered data particularly at small strains and near their extremum values, and the absence of sharp corners of the hysteresis curves are addressed. The parameters determined with the improved procedures then are implemented into an ABAQUS-model of a specimen for S235 steel, and good coincidence with experimental results is shown.

[1] G. Mastinu, M. Plöchl. Road and Off-Road Vehicle System Dynamics Handbook (CRC Press, Taylor and Francis, Boca Raton, 2014).

[2] K.H. Nip, L. Gardner, C.M. Davies, A.Y. Elghazouli. Extremely low cycle fatigue tests on structural carbon steel and stainless steel, J. Construct. Steel Res. 66 (2010), 96-110.

[3] H. Badnava, S.M. Pezeshki, Kh. F. Nejad, H.R. Farhoudi. Determination of combined hardening material parameters under strain controlled cyclic loading by using the genetic algorithm method, J. Mech. Sci. and Technol. 26 (2012), 3067-3072.

[4] ABAQUS user's manual.

[5] J. Shit, S. Dhar, S. Acharyya. Experimental and numerical simulation of carbon manganese steel for cyclic plastic behaviour, Int. J. Eng., Sci. Technol. 2 (2010), 71-84.

Identification of inelastic material parameters using component-oriented specimen with design of experiments

N. Nostitz (German Institute of Rubber Technology), N. Kröger (German Institute of Rubber Technology), J. Ihlemann (Chemnitz University of Technology) 14:20

To guarantee a realistic simulation of a component, a well chosen material model is needed. Therefore, a parameter identification is necessary because a more realistic material model requieres more material parameters. The common procedure is the comparison between simulations and selected experiments, where the usage of standard test specimen has been established.

Due to the fact that standard test specimen very often represent homogeneous experiments, an alternative test specimen should be used because the component is mostly inhomogeneous. The theoretical best alternative would be the usage of the original component to identify the parameters. However unfortunately this isn't efficient due to the computational effort of the FEM-simulations for a whole parameter optimization. Hence, a compromise between both options has to be chosen: the component-oriented specimen.

For this work, a bushing as the original component with typical load cases: axial, radial, torsional and cardanic was chosen. For the comparison the Yeoh model and the Model of Rubber Phenomenology (MORPH) are used. A component-oriented specimen with less complicated geometry and identical manufacturing process was designed. To guarantee practical results, the stress-strain curves of the simulations of the identified material parameters of the standard test specimen and the ones of the component-oriented specimen were checked by the original component. The MORPH-parameter set of the component-oriented specimen yields much better results than the one of the standard test specimen set and fits the component behavior well.

The parameter identification process is done by using the Levenberg-Marquardt-Fletcher algorithm. One disadvantage of such an algorithm is its convergence to the next local minimum, which isn't necessarily the global minimum. An additional design of experiments supports the search of the best existing parameter set. Therefore, two material models are used to verify the importance of the initial parameter set.

Application of Identifiability in Solid Mechanics

S. Hartmann (Technische Universität Clausthal), R. Gilbert (Technische Universität Clausthal) 14:40

Material parameter identification is a wide spread method to calibrate a constitutive model to experimental data. Commonly, least square methods are applied. The simulation can be very simple algebraic equations, systems of ordinary equations, or even entire finite element programs to consider the underlying boundary-value problem. The result of identification can be qualified by the R^2,-value, the variance, the correlation

and the confidence interval. Additionally, one should investigate whether the parameters can be determined by the given data or not. This is related to the notion of identifiability. In this presentation, identifiability is discussed for the simplest cases of isotropic elasticity in the field small and finite deformation, where simple tension, biaxial deformation, thick-walled tubes under internal pressure, bending, and ball indentation are possible. The investigations take into consideration the possibilities to incorporate more information using full-field displacement fields.

Determination of material parameters for a sheet-layered lamination stack

M. Baloglu (FAU Erlangen-Nürnberg), K. Willner (FAU Erlangen-Nürnberg) 15:00

For the numerical FE-simulation of sheet-layered lamination stacks, which can be found in transformers or in electric motors as rotor and stator, it is necessary to use a material model, which covers the special microstructure of such components. Depending on the manufacturing process, these sheets are either linked together with the help of a bonding varnish or just packed up and in contact to each other such that they are basically free to slip inside of the stack and show a nonlinear deformation behavior. Even though the neglection of individual sheet interaction may lead to inappropriate results, a FE-discretization incorporating all interlayers is not desirable in terms of performance as well as computational effort and often not feasible for realistic problems with hundred of thin sheets. Therefore, numerical homogenization is utilized to identify a sophisticated material model to cover the real physical behavior of a lamination stack in an efficient and accurate way, as presented in [1] and [2].
It can be assumed that the material is orthotropic, more precisely transversely isotropic and has therefore one preferred direction, in which the stress-strain relation differs significantly from the other two directions. For this special case, only five independent parameters have to be determined to derive a (linearized) material law, e.g. in the form of Hooke's law. By applying different load cases, the elasticity tensor, which defines the stress-strain relation, can be identified and linearized at an operating point as shown in [3] for different pretensions of the stack.

[1] Vera Luchscheider: *Experimentelle und numerische Identifikation eines homogenisierten Materialmodells für Blechpakete elektrischer Maschinen.* PhD thesis, Friedrich-Alexander-Universität Erlangen-Nürnberg, 2016.

[2] M. Volkan Baloglu and Kai Willner: *Material modelling of a sheet-layered lamination stack by homogenization.* In *PAMM*, Vol. 16. Wiley Online Library, pp. 509–510, 2016.

[3] M. Volkan Baloglu and Kai Willner: *Numerical homogenization and simulation of a lamination stack.* In 6^{th} *International Electric Drives Production Conference (EDPC)*. IEEE, pp. 67–72, 2016.

Basic Ideas for the Quantification of Uncertainty Associated with the Material's Microstructure Morphology using Statistically Similar RVEs

N. Miska (Institute of Mechanics and Shell Structures, TU Dresden), S. Prüger (Institute of Mechanics and Shell Structures, TU Dresden), D. Balzani (Dresden Center for Computational Materials Science (DCMS)) 15:20

Advanced high strength steels combine a high ductility with high strength. The macroscopic response of these steels is governed by a pronounced microstructure, whose morphology varies over the location in the macroscopic part and over different specimen. This randomness of the microscopic morphology implies uncertainties regarding the macroscopic material response. We propose to create statistically similar representative volume elements (SSRVE), cf. [1], to enable access to the incorporation of these uncertainties in numerical computations. The SSRVEs are the result of an optimization of higher order statistical measures, which describe the morphology of the microstructure. The resulting geometries are significantly less complex than the real microstructure and therefore advantageous with view to the computational effort required for meshing and computing the problem. Beside these advantages, the main intent of using this method here is to provide a basis to construct various SSRVEs which are within predefined bounds regarding the microstructure statistics. These bounds may be obtained from measurements performed by analyzing the microstructures at different locations in one material. Based on this variety of applicable SSRVEs, multiple Finite Element (FE) simulations can be performed to obtain the homogenized response and thus, to quantify statistics regarding macroscopic material parameters. In order to automatize these numerical simulations, the Finite Cell Method (FCM) can be applied such that a conforming FE mesh for each SSRVE are avoided.

[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.

Material based process chain optimization in metal forming

L. Morand (Karlsruher Institut für Technologie), J. Pagenkopf (Fraunhofer-Institut für Werkstoffmechanik IWM), D. Helm (Fraunhofer-Institut für Werkstoffmechanik IWM) 15:40

The process chain in metal forming consists of several process steps leading to a final product with specific characteristics influenced by a variety of different factors. For the optimization of the process chain, an inverse view of its individual steps is essential. In contrast to the direct problem, which is based on a predetermined sequence of cause and effect, the inverse modelling tries to infer from the desired characteristics of the final product to the required properties of the starting product. The present work concentrates on the representation of polycrystalline microstructure of metals, which has a high impact on the deformation behavior of the material during a process step. Using methods of machine learning (neural networks) a solution of the inverse problem can be realized. The aim of this work is to present an approach for the inverse problem formulation of the process chain. Due to the ill-posed nature of this problem, we will

consider questions that arise regarding a single crystal such as the ambiguity of the crystal orientation. Furthermore, the identification of the reachable states in metal forming and their limiting character to neural network prediction will be discussed.

S 6a : Material modelling in solid mechanics

Wednesday 16:30 - 18:30 Marienstr. 13, 1st floor, Lecture hall B
Chair: Mikhail Itskov (RWTH Aachen)
Ralf Landgraf (TU Chemnitz)

Estimation of the compression modulus of a technical EPDM via cyclic volumetric compression tests

O. Gehrmann (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany), N. Kröger (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany), P. Erren (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany), D. Juhre (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany) 16:30

In many applications for finite-element (FE) simulations rubber materials are assumed to be nearly incompressible by applying a high ratio between compression modulus and shear modulus. The compression modulus is commonly a constant value for FE analyses. The focus of this work is on the estimation of the cyclic evolution of the compression modulus for a technical EPDM by using cyclic volumetric compression tests.
By post-treating the global reaction force and global displacement, material softening (with repeated loading) and a distinct hysteresis loop can be observed. These effects are often observed and well known for filled rubbery materials exposed to cyclic non-hydrostatic loadings. The loading of the specimen in the realized compression test is considered to be hydrostatic. That assumption is proven with an analytical investigation of the test procedure. Looking more closely on the compression modulus it can be shown that this modulus is significantly a function of loading intensity and loading history. Finally first statements are formulated to explain the observed material behavior.

Considering time- and temperature-dependent effects of elastomers within the Model of Rubber Phenomenology

N. Kröger (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany), R. Raghunath (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany), J. Plagge (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany) 16:50

Filled elastomers are showing not only pronounced material softening and moderate inelastic behavior, e.g. Mullins and Payne effect, but also creep and relaxation phenomena can be observed.

Common material models to characterize the complex behavior of those elastomers are for example the MOdel of Rubber PHenomenology (MORPH) and the Dynamic Flocculation Model (DFM). In general, one neglects the time- and temperature-dependent effects and conducts experiments for characterization for modes which are quasi-static. With higher velocity in tension tests and especially with increasing filler content, the contribution of time-dependent effects is well pronounced and neglecting them is no longer reasonable. The rate-dependent effects as well as relaxation phenomena are well-known to be temperature-dependent as well.

In this paper we present a modelling approach for thermo-viscohyperelasticity based on previous works which extended the MORPH to viscous effects. This extension is realized via a Prony-Series approach. Hereby, a functional dependency of the relaxation times and their weights is assumed. In order to cover temperature-dependent effects as well, a WLF ansatz is included. The model is validated via experimental data for different strain-rates in several isothermal test environments.

Phenomenological modelling of curing phenomena in a PU based adhesive

R. Landgraf (Chemnitz University of Technology), J. Ihlemann (Chemnitz University of Technology) 17:10

In this contribution, the phenomenological material modelling of a polyurethane based adhesive including the curing process is considered. The initial paste-like adhesive includes encapsulated isocynate which gets released at temperatures above 85°C. Once the curing reaction has started, the process to complete solidification only takes few minutes. The final material exhibits rubber-like mechanical behaviour.
To characterize the curing process, differential scanning calorimetry tests as well as torsional rheometer tests were carried out. Moreover, uniaxial tension tests with cyclic and quasi-static loading scenarios on the fully cured material were conducted and revealed typical behaviour of elastomers, like Hysteresis, Mullins effect and permanent set. Based on the experimental results, a constitutive model has been formulated to capture the mechanical behaviour of the material in the fully cured state as well as within the curing process. To this end, a phenomenological description of the degree of cure is included. The modelling approach is based on the general curing model [2] as well as the phenomenological model [1] for the representation of rubber like materials.

[1] Ihlemann, J. (2003). Kontinuumsmechanische Nachbildung hochbelasteter technischer Gummiwerkstoffe. VDI, Düsseldorf.

[2] Landgraf, R. (2016). Modellierung und Simulation der Aushärtung polymerer Werkstoffe. Verlag Dr. Hut, München.

A network model of dielectric elastomers based on molecular chain statistics

M. Itskov (RWTH-Aachen University), V. Khiêm (RWTH Aachen University), S. Waluyo 17:30

An electric field imposed on a dielectric elastomer causes mechanical stress or strain without any applied load. The latter phenomenon is referred to as electrostriction. There are many phenomenological models describing this electro-active response of dielectric elastomers. In this contribution, we proposed an electro-mechanical constitutive model based molecular chain statistics. The model considers polarization of single polymer chain segments and takes into account their directional distribution. The latter one results from the non-Gaussian chain statistics taking finite extensibility of polymer chains into account. The so resulting electric potential of a single polymer chain is further generalized to the network potential serving as a basis for the prediction of the above mentioned electro-active response.

On a relaxation approach to modeling the stochastic behavior of elastic materials

P. Junker (Institute of Continuum Mechanics, Ruhr-Universität Bochum), J. Nagel 17:50

Even in the simple linear elastic range, the material behavior is not deterministic, but fluctuates randomly around some expectation values. The knowledge about this characteristic is obviously trivial from an experimentalist's point of view. However, it is not considered in the vast majority of material models in which "only" deterministic behavior is taken into account.

One very promising approach to the inclusion of stochastic effects in modeling of materials is provided by the so-called Chaos Polynomial Expansion. It has been used, for example, to derive the so-called stochastic finite element method. This method yields results that are exactly of the desired kind, but unfortunately at drastically increased numerical costs.

This contribution aims to propose a new ansatz that is also based on a stochastic series expansion at the Gauß point level. Appropriate energy relaxation provides a synthesized (deterministic) stress measure, while simultaneously offering stochastic properties such as the variance. The total procedure only needs negligibly more computation effort than a simple elastic calculation.

A physically motivated model based on the strain amplification factor in filled elastomers

E. Darabi (Department of Continuum Mechanics, RWTH Aachen University), M. Itskov (Department of Continuum Mechanics, RWTH Aachen University), M. Klüppel (Deutsches Institut für Kautschuktechnologie e.V., Hannover, Germany) 18:10

A constitutive model for filled elastomers based on a combination of the Dynamic Flocculation Model (DFM) [1] framework and the continuum damage model [2] is proposed. This contribution represents an extension of the previously proposed micro-mechanical model explaining simultaneously induced filler breakage and polymer-filler network damage [3]. These effects are attributed to the hydrodynamic strain amplification which is the main topic of the current work. Deformation causes damage in both the network

rubbery matrix and inside the filler aggregates. As a result, the probability density function of the number of segments and the filler size distribution change with the strain in all spatial directions which leads to stress softening and the Mullins effect. The model also describes the deformation induced anisotropy and permanent set. A small number of physically motivated material constants describing the average filler cluster dimensions, filler-filler and filler-matrix interaction properties are included in the model.

[1] Klüppel, M. *Advances in Polymer Science* 2003, 164, 1-86.

[2] Govindjee, S.; Simo, J. *Journal of the Mechanics and Physics of Solids* 1991, 39, 87-112.

[3] Darabi, E.; Itskov, M.; Klüppel, M. *PAMM* 2016, 16, 315-316.

S 6b : Material modelling in solid mechanics

Wednesday 16:30 - 18:30 Marienstr. 13, 1st floor, Lecture hall D

Chair: Steven Becker (TU Kaiserslautern)
Robert Bischof (TU Kaiserslautern)

Numerical investigations of CMC nozzle structures: constitutive modelling and finite element technology

O. Barfusz, M. Schwarze, S. Reese (Institute of Applied Mechanics, RWTH Aachen University) 16:30

This work deals with the development of numerical tools predicting the lifetime of nozzle structures made of carbon fibre reinforced ceramic matrix composites (CMC). These materials are favorable for thermostructural components due to their excellent specific mechanical properties, high thermal conductivity and thermoshock resistance. The anisotropic constitutive behaviour of the CMC is reflected by a continuum model which is micro-mechanically motivated. The model is based on structural tensors [1] representing different fibre orientations. Furthermore, the thin structure of the nozzle requires an appropriate finite element technology in order to overcome locking phenomena. For this reason, a solid-shell formulation with reduced integration [2] is utilized, for which the implementation of the material/fibre orientation is crucial. The enhanced assumed strain (EAS) concept is used to avoid volumetric locking as well as Poisson thickness locking. The transverse shear and curvature thickness locking are cured by the assumed natural strain (ANS) concept. Using reduced integration together with hourglass stabilization leads to high computational efficiency.

[1] S. Reese, T. Raible, P. Wriggers, International Journal of Solids and Structures 38, pp. 9525–9544, 2001.

[2] M. Schwarze, S. Reese, International Journal for Numerical Methods in Engineering 85, pp. 289–329, 2012.

On Modeling of Thermo-Viscoplasticity of Case-Hardening Steels Over a Wide Temperature Range

P. Oppermann (Lund University / LTH), R. Denzer (Lund University / LTH), A. Menzel (Lund University / LTH) 16:50

The aim of this work is the development of a thermodynamically consistent fully coupled thermo-viscoplastic material model for metals. The model is based on a split of the free energy into a thermo-elastic, a thermo-plastic and a purely thermal part and covers nonlinear cold-work hardening and thermal softening. Nonlinear temperature dependent effects are accounted for the elastic moduli, the plastic hardening moduli, the thermal expansion, the heat capacity and the heat conductivity. Furthermore strain rate-dependency of the current yield stress is realized using a temperature dependent nonlinear Perzyna-type viscoplastic model. The model and its parameters are fitted against experimental data for case hardening steel 16MnCr5 (1.7131). Since for some constitutive parameter sets describing thermal softening the model may result in unphysical behaviour, we introduce necessary conditions to check the thermodynamical admissibility of these parameters. We discuss the consistent linearisation of the proposed model and its implementation in a monolithic fully coupled finite element framework. Finally, we present results for selected boundary value problems. These show the localization and regularisation behaviour of the proposed model.

Finite Element Simulation of the Temperature Evolution during Cryogenic Turning

S. Becker (University of Kaiserslautern), P. Mayer, H. Hotz, B. Kirsch, J. Aurich, E. von Harbou, R. Müller (TU Kaiserslautern) 17:10

In order to shorten the process chain in manufacturing and thus to optimize the manufacturing time, current researches investigate the possibility of combining two process steps, turning and hardening.

During cryogenic turning metastable austenitic steel, deformation induced hardening in the surface layer of the workpiece can be achieved by applying high passive forces onto the workpiece [3]. This leads to an increase in the wear resistance [2] as well as the fatigue strength [2]. For the employed austenite-martensite phase transformation it is necessary to maintain low process temperatures, typically below room temperature. Thus, cryogenic cooling has to be applied to counteract the heat, generated while machining [6].

For a better understanding of the influence of different cutting and cooling parameters on the temperature field during cryogenic turning, and thus martensite formation, knowledge of the exact temperature distribution in the workpiece and the workpiece surface temperature in the contact zone is essential. Since in situ measurements of the latter are hardly possible, an inverse determination via transient finite element simulation is

performed [5].
In order to model cryogenic turning, thermal loads and material properties, i.e. heat transfer coefficients defining convective heat transfer, have to be determined first. Therefore they are investigated independently in stand-alone experiments, applying only one thermal load at a time. The magnitudes of these values are obtained by iteratively modifying the initial values in the model until correspondence with measured temperature data from the experiment is achieved.
The present finite element approach only takes thermal loads into account and is performed in the finite element program FEAP (Finite Element Analysis Program) with an Eulerian mesh, which requires special consideration of the rigid body rotation of the workpiece. The Eulerian treatment results in an unsymmetrical system matrix, and a special stabilisation is required to avoid numerical oscillations in the time integration scheme.

[1] J.C. Aurich, P. Mayer, B. Kirsch, D. Eifler, M. Smaga, R. Skorupski. Characterization of deformation induced surface hardening during cryogenic turning AISI 347. CIRP Ann. – Manuf. Technol. 2014; 63/1:65–68

[2] D. Frölich, B. Magyar, B. Sauer, P. Mayer, B. Kirsch, J.C. Aurich, R. Skorupski, M. Smaga, T. Beck, D. Eifler. Investigation of wear resistance of dry and cryogenic turned metastable austenitic steel shafts and dry turned and ground carburized steel shafts in the radial shaft seal ring system. Wear 328–329 (2015), 123–131.

[3] R. Skorupski, M. Smaga, D. Eifler. Influence of surface morphology on the fatigue behavior of metastable austenitic steel. Adv. Mater. Res. 2014; 891–892:464–469.

[4] P. Mayer, R. Skorupski, M. Smaga, D. Eifler, J.C. Aurich. Deformation induced surface hardening when turning metastable austenitic steel AISI 347 with different cryogenic cooling strategies. Procedia CIRP 2014; 14:101–106.

[5] S. Becker, P. Mayer, B. Kirsch, J.C. Aurich, E. v. Harbou, R. Müller. Transient Finite Element Simulation of the Temperature Field during Cryogenic Turning of Metastable Austenitic Steel AISI 347. Proc. Appl. Math Mech. 2016; 16:303–304.

Robust implementation of multi-slip crystal plasticity for micro machining simulations (based on Fischer-Burmeister complementary functions)

R. Bischof (TU Kaiserslautern), F. Schneider (TU Kaiserslautern), C. Müller (TU Kaiserslautern), C. Kuhn (TU Kaiserslautern), J. Aurich (TU Kaiserslautern), R. Müller (TU Kaiserslautern) 17:30

As opposed to conventional machining processes, the crystalline structure of commercially pure (cp) titanium plays an important role in micro machining processes [1]. Suitable simulation techniques are important to get insight into the process mechanisms on the microscale and to support the improvement of the manufacturing process. Finite element simulations of micro machining processes involve several challenges, since the

workpiece material undergoes large deformations during chip formation and eventually material separation needs to be modeled.
A robust implementation of the finite deformations multi-slip crystal plasticity model describing the material response of the hexagonal close packed-structured cp-titanium is the basis for such simulations. One challenge in the implementation of multi-slip crystal plasticity is the determination of the active set of plastic slip systems. Standard predictor corrector formulations based on Karush-Kuhn-Tucker (KKT) conditions often fail, because the active set cannot always be determined from the predictor step and additional selection criteria need to be formulated [2]. In order to circumvent the explicit determination of the set of active slip systems, the KKT conditions can be replaced by a system of Fischer-Burmeister complementary functions [3]. Simulations demonstrate that this formulation implicitly selects the correct set of active slip systems and improves the stability of the simulations.

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Numerical implementation of general imperfect interface models at finite deformations accounting for material degradation

T. Heitbreder (Institute of Mechanics, TU Dortmund), N. Ottosen (Lund University / LTH), M. Ristinmaa (Lund University / LTH), J. Mosler (Institute of Mechanics, TU Dortmund) 17:50

Cohesive zone models are well established and frequently applied for the numerical analysis of material failure. However, considering a geometrically exact description (finite deformation), fundamental principles such as balance of angular momentum [2], material frame indifference and thermodynamical consistency [1] are only fulfilled in the classical cohesive zone framework, if the traction vector is colinear to the displacement jump, i.e. these models have essentially to be fiber models. This constrains the ability to model shear and anisotropic effects are excluded in general. Within this talk, the numerical implementation of the novel extended framework for cohesive zone models [3], which is consistent with the above mentioned fundamental physical principles, is presented. In addition to anisotropic hyperelasticity, anisotropic material degradation is also accounted for. The resulting model and its implementation are finally embedded

within an FE2-type homogenization scheme in order to analyze the effect of general imperfect interfaces on the overall mechanical response. REFERENCES [1] J. Mosler, I. Scheider, “A thermodynamically and varationally consistent class of damage-type cohesive models”, Journal of the Mechanics and Physics of Solids, 59, 1647-1668, (2010). [2] N.S. Ottosen, M. Ristinmaa and J. Mosler, “Fundamental physical principles and interface models at finite displacements – Limitations and possibilities”, International Journal of Solids and Structures, 53, 70-79, (2015). [3] N. S. Ottosen, M. Ristinmaa and J. Mosler, “Framework for non-coherent interface models at finite displacement jumps at finite strains”, Journal of the Mechanics and Physics of Solids, 90, 124-141, (2016).

Modeling and simulation of the thickness dependence in zinc die casting structures

M. Martinez Page (Technische Universität Clausthal), M. Ruf (Technische Universität Clausthal), S. Hartmann (Technische Universität Clausthal) 18:10

Several die casting materials, for example zinc die casting alloys, show different mechanical responses for specimens with different thicknesses. This can be observed in the variation of parameters, such as the Young’s modulus, the tensile strength or hardness of the material, with the thickness. The origin of this thickness dependence can be found in the microstructure of the material and the void distribution, which changes through the thickness of the specimen because of the temperature distribution during solidification step of the die casting process. One example of a microstructural change over the thickness of the specimen is the porosity, which is a very common defect in die casting materials. In previous investigations, it has been observed that the porosity is higher in the middle of the thickness of the specimen and it decreases approaching the surface. A thicker specimen possesses a larger area with a higher porosity than a thin one and has therefore a lower effective area.

In this presentation, we propose a method to model the influence of the porosity distribution over thickness in a zinc die casting alloy. To this end, some experimental observations about the porosity distribution in a zinc die casting specimen are shown first. In the modeling part, a structural parameter κ is introduced in order to model the microstructural change through the thickness. This parameter is a dimensionless scalar with values between 0 (surface of the specimen) and 1 (saturation value) and develops following a partial differential equation. The porosity is defined in dependence of the structural parameter. Moreover, the influence of the porosity in the model is presented and a parameter identification is carried out. Finally, we present the behavior of the model with the help of different finite element simulations.

S 6a : Material modelling in solid mechanics

Thursday 14:00 - 16:00 Marienstr. 13, 1st floor, Lecture hall B

Chair: Simon, R. Eugster (Universität Stuttgart)
Fadi Aldakheel (Universität Stuttgart)

A Phase field model for studying anisotropic volume strain during lithiation of Silicon nanowires

M. Al- Siraj (TU Darmstadt), Y. Zhao, P. Stein (TU Darmstadt), B. Xu (TU Darmstadt) 14:00

Pushing the edges of storage capacity and reliability of Li-ion batteries remains in focus of current research activities as it requires incorporation of novel materials and design to exploit the full potential of renewable energy sources. Demand now seeks new materials with higher Li-storage capacity, more environment friendly and higher safety margin than conventional materials for construction. For anode, Si-based materials possess all such desirable properties [1] and hence, has been under investigation recently to predict their behavior under battery operation condition. Several key factors of Si-based materials remain challenging like high volume expansion ($\sim 400\%$), low electrical conductivity and capacity fade due to damage from strain and continuous SEI formation. To solve such issues, nano structured Si and composite Si-based electrode materials are also studied [2].

It has been confirmed from several in-situ experiments that lithiation in Si Nano Wires (NW) is accompanied with a sharp interface between Li-rich amorphous shell and Li-poor crystalline core. Additionally, the volume expansion (or swelling) from lithiation in amorphous region is reported to be anisotropic. For example, along <110> direction the expansion is high [$\sim$170%] and along <111> direction, it is low [only $\sim$ 20%]. The origin and consequences of such behavior was under study based on the first-principles [3], atomistic simulations [4], and continuum model [1].

We present a model with such anisotropic expansion effects in the framework of a mechanically coupled Cahn-Hilliard phase field model by incorporating anisotropic diffusivity. The parameters of the model results from the atomistic simulations results. Additionally, we will focus on the interplay between the anisotropic interface evolution and the resulting mechanical behavior in different Si nano wires. 2D simulation model will be used for analysis of the anisotropic behavior on different cross sections.

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Phase Field Modeling of Ductile Fracture in Soil Mechanics

F. Aldakheel (Institute of Applied Mechanics (CE)), D. Kienle (University of Stuttgart), M. Keip (University of Stuttgart) 14:20

This work outlines a rigorous framework for the ductile failure of frictional materials in elastic-plastic soil mechanics undergoing large strains. Describing soil crack formation can be achieved in a convenient way by recently developed continuum phase field approaches to fracture, which are based on the regularization of sharp crack discontinuities [1]. This avoids the use of complex discretization methods for crack discontinuities, and can account for complex crack patterns. For frictional materials, a *non–associative* Drucker–Prager–type elastic-plastic constitutive model suitable for a wide range of applications in soil mechanics is developed [2], and linked to a failure criterion in terms of the elastic-plastic work density that drives the fracture phase field. On the algorithmic side, we develop a general return mapping scheme of the non–associative elastoplasticity in the spectral space of logarithmic principal strains and dual stresses. We demonstrate the modeling capabilities and algorithmic performance of the proposed formulation by representative simulations that describe soil crack formation using elastic-plastic fracture mechanics.

[1] C. Miehe, M. Hofacker and F. Welschinger. A phase field model for rate-independent crack propagation: Robust algorithmic implementation based on operator splits. *Computer Methods in Applied Mechanics and Engineering*, 199:2765–2778, 2010.

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A phase-field model of ductile fracture incorporating viscoplasticity

L. Zhang (Institute of General Mechanics, RWTH Aachen University), B. Markert (Institute of General Mechanics, RWTH Aachen University) 14:40

Ductile fracture occurs in plastic areas and ensures a mesh objectivity in the aspect of computation in post-critical ranges [1]. The accumulation of the plastic deformation leads to the crack propagation. A viscoplastic constitutive formulation should be used to describe the behaviour of the material. The large strain framework is assumed to be justified by the domain of application to cyclic loading condition. The ductile fracture is represented by a phase-field model, which is limited of the sharp interface and replaced by a diffuse-interface model.

The phase-field method makes the simulation of the fracture problem much simpler, since it eliminates the demands of the numerical tracking of discontinuities in the displacement field compared to discrete damage methods [2]. The phase-field approach benefits from abstaining the complex geometry structure and meshing. Furthermore, it can simulate multiple initial cracks, branching and propagation in complex constructions. The present work is to couple the phase-field method and the mesoscale viscoplastic model accounting for a framework of the mechanics similar to the one previously in [3]. To this end, a phase-field model is implemented for simulating ductile fracture in the Abaqus software as user subroutines (UMAT and UEL) based on a viscoplastic constitutive framework.

Key words:

phase-field model; Abaqus user subroutines; viscoplasticity; finite element method

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Boundary integral equation method in the theory of thermoelasticity for triple porosity materials

M. Svanadze (Ilia State University) 15:00

This paper concerns with the full coupled linear theory of thermoelasticity for triple porosity materials. The system of the governing equations based on the equations of motion, conservation of fluid mass, the constitutive equations, Darcy's law for materials with triple porosity and Fourier's law of heat conduction. The system of equations of motion is expressed in terms of the displacement vector field, the pressures in the three pore systems and the temperature.

In this talk the 3D basic boundary value problems (BVPs) of steady vibrations of the theory of thermoelasticity for materials with triple porosity are investigated. The representations of general solutions for the system of equations of steady vibrations and the Green's formulae in the considered theory are obtained. The Sommerfeld-Kupradze type radiation conditions are established and the uniqueness theorems for solutions of the BVPs of steady vibrations are proved. The basic properties of surface and volume potentials are established. On the basis of boundary integral equations method and the theory of singular integral equations the existence theorems for solutions of the BVPs of steady vibrations are proved.

Acknowledgments.
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Boundary value problems in the theory of thermoviscoelasticity for double porosity materials

M. Svanadze (Tbilisi State University) 15:20

Viscoelastic materials play an important role in many branches of engineering, technology and biomechanics. In the last decade there has been interest in formulation of the mechanical theories of viscoelastic and thermoviscoelastic materials with microstructures of differential type.

In the present paper the linear theory of thermoviscoelasticity for Kelvin-Voigt materials with double porosity is considered. The fundamental solutions of the systems of equations of steady vibrations and quasi statics are constructed by means of elementary

functions and their basic properties are established. The representation of Galerkin type solution is obtained. The formulas of representations of the general solutions for the system of homogeneous equations of steady vibrations and quasi statics in terms of elementary functions are established. The completeness of these representations of solutions is proved. The uniqueness theorems of the internal and external basic boundary value problems of steady vibrations and quasi statics are proved. The Green's formulas and integral representations of Somigliana type of regular vector and classical solution are obtained. The basic properties of surface and volume potentials and singular integral operators are established. Finally, the existence theorems for classical solutions of the above mentioned BVPs are proved by using the potential method (boundary integral equation method) and the theory of singular integral equations.

Acknowledgments
This research has been fulfilled at Ilia State University (Tbilisi, Georgia) by financial support of Shota Rustaveli National Science Foundation (Grant # FR/18/5-102/14).

An ignored source in the foundations of continuum physics "Die Allgemeinen Ansätze der Mechanik der Kontinua" by E. Hellinger

S. Eugster (University of Stuttgart), F. dell'Isola 15:40

In 1913 Ernst Hellinger finished his remarkable article DIE ALLGEMEINEN ANSÄTZE DER MECHANIK DER KONTINUA, which appeared in German language in the "Encyklopädie der mathematischen Wissenschaften mit Einschluss ihrer Anwendungen". Following his predecessors J.-L. Lagrange, G. Piola and the Cosserat brothers, Hellinger presents in this paper a nonlinear field theory of continuum physics entirely based on a variational principle "the principle of virtual displacements". Even though Hellinger focuses on the fundamentals of continuum mechanics, he presents within the very same variational framework the physics of optics, electrodynamics, thermodynamics and the theory of relativity. Accordingly, Hellinger's paper can be understood as a contribution to continuum physics in general. However, due to the establishment of English as the upcoming scientific language and due to the refusal of a variational formulation of continuum mechanics in the subsequent period, Hellinger's contribution to the foundations of continuum physics has been ignored for decades and has almost fallen into oblivion. In order to steer in the opposite direction, recently an English translation of Hellinger's masterpiece has been made available by the authors of this paper. In reading Hellinger, one obtains astonishing facts concerning the scientific development of mechanical sciences. Already in 1913, Hellinger was completely aware of media with oriented particles, higher-gradient theories, space-time formulations of continuum dynamics and much more. A remarkable discovery among others is the concise statement of the principle of material frame-indifference for constitutive equations for stress.
In this paper, we discuss some insights reached by Hellinger in the mathematical structure of continuum physics which seems, in some aspects, unsurpassed even nowadays. Special emphasis is placed on the variational formulation of continuum mechanics which still seems to be controversial.

S 6b : Material modelling in solid mechanics

Thursday 14:00 - 16:00 Marienstr. 13, 1st floor, Lecture hall D
Chair: Markus Bambach (BTU Cottbus - Senftenberg)
Thorsten Bartel (TU Dortmund)

Towards a micromagnetics-inspired framework for the modelling of variant switching in magnetic shape memory alloys under inhomogeneous conditions

T. Bartel (TU Dortmund), B. Kiefer (Technische Universität Bergakademie Freiberg), K. Buckmann (TU Dortmund), A. Menzel (TU Dortmund) 14:00

The aim of our contribution is the application of quasiconvex analysis — which has so far already beneficially been used in the context of conventional shape memory behaviour — to magnetomechanically coupled constitutive behaviour as occurring in ferromagntic materials and, more precisely speaking, magnetic shape memory alloys (MSMA). The point of departure is an energy functional which depends on three global field variables, namely the displacement field, the magnetic potential, and the magnetisation. This functional is chosen such that the Euler-Lagrange equations obtained via variational calculus yield the mechanical equilibrium conditions, the Gauß-Faraday law, the respective Neumann boundary conditions, and a constitutive relation between the total magnetic field and the magnetisation. This approach — inspired by theories from the field of micromagnetics — works well in cases where, e.g., the energy associated with the demagnetisation field can be obtained by the introduction of a demagnetisation tensor, and a phenomenological model for the internal magnetic energy stored in the material depending on the magnetisation is used. However, in our approach, the magnetisation is explicitly dependent on internal state variables associated with the quasiconvexification of the nonconvex elastic energy density, which causes specific flaws in the present framework. More precisely speaking, the feedback between the global field variables and the purely local variables does not occur as desired in the general case. In our presentation, we provide general solution strategies to overcome these shortcomings.

Consistency of dynamic recrystallization models from the perspective of physical metallurgy and continuum mechanics

M. Bambach (BTU Cottbus - Senftenberg), S. Klinge (TU Dortmund University) 14:20

Dynamic recrystallization (DRX) is characterized by the nucleation and growth of new grains, which takes place concurrently to plastic deformation. DRX processes are used in industrial hot forming processes to control the microstructure and properties of the workpiece. Various models have been developed that consider the coupled evolution of microstructure and flow stress during hot deformation processes, some from a perspective of physical metallurgy, some from continuum mechanics. It is widely accepted that the onset of DRX is characterized by an inflection point of the strain hardening rate as

a function of stress. This criterion was derived by Poliak and Jonas [1] using results from the thermodynamics of irreversible processes. The present talk analyses different existing DRX models, both from physical metallurgy and continuum mechanics, for consistency with the criterion by Poliak and Jonas. It is shown that for models which use classical Avrami kinetics to describe the evolution of the recrystallized volume fraction, the Avrami exponent should exceed a value of 3 to ensure that the Poliak-Jonas criterion is not violated. Based on this observation, a consistent framework for DRX models is presented and discussed.

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Influence of Dissipation on the Formation of Striations in Single Crystals under Simple Shear Deformation

M. Koster (Ruhr-Universität Bochum), K. Le (Ruhr Universität Bochum) 14:40

Aluminum single crystals exposed to equal-channel angular pressing (ECAP) show different regions, where the formation of striations of various orientations can be observed, depending on the initial orientation of the crystal's slip systems [2, 3].
In order to capture some of the basic features seen in real crystals a model describing laminate formation in single crystals with a single active slip system taking into account dissipation is proposed for the case of plane strain simple shear deformation. To describe plastic deformation of single crystals the framework of nonlinear continuum dislocation theory (CDT) [5] is used. All pertinent equations and conditions defining a first-order laminate structure using CDT are obtained using the variational principle of minimum of the energy applied to a crystal containing a surface of discontinuity [5]. As the energy density function of the material is non-convex this allows for the construction of a lamellar structure mixing two energy states [1] where laminate layers have deformation properties related to each state. Depending on the assumed value of the critical resolved shear stress, which is introduced in the model through the dissipation function, the properties of the laminate change. It can be found that in a certain range of orientations of the slip system non-convexity of the energy is present. For these orientations it turns out that elastic deformations are pure rotations of the crystal lattice in the case where dissipation is neglected.
The influence of the variation of the slip system orientation and the value of the critical resolved shear stress on the resulting laminate structure is investigated and compared to the findings from experiments on high purity aluminum single crystals with different slip system orientations in ECAP processing.

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Multiscale modeling of thermoplastic PC/ABS blends

J. Hund (Karlsruher Institut für Technologie (KIT)), T. Seelig (Karlsruher Institut für Technologie (KIT)) 15:00

J. Hund, Th. Seelig
Institute of Mechanics, KIT

Rubber-toughened thermoplastic polymer blends such as PC/ABS exhibit a pronounced plastic dilatancy in their overall deformation behavior. This volume increase results from different damage mechanisms (void growth, crazing) which prevail primarily in the ABS phase, e.g. [1].
In this contribution, a micromechanical RVE approach modeling the two constituents PC and ABS as two distinct phases is presented. This approach features different plasticity models to capture the different deformation behavior of each phase. Numerical cell model studies looking at the effect of the blend composition on the overall response are compared with experimental data.
Furthermore, macroscopic material models featuring overall plastic dilatancy are analyzed with respect to their capability to match experimental data for PC/ABS blends. This comprises finite element simulations of fracture experiments and the comparison with experimental results.

[1] Van der Giessen, E., Seelig, Th., 2015. Computational modeling of rubber-toughening in amorphous thermoplastic polymers - a review. *Int. J. Frac.* **196**, 207-222

Constitutive modeling of mechanoluminescence based on the analytical network-averaging concept

V. Khiêm (RWTH Aachen University), M. Itskov (RWTH Aachen University) 15:20

One of the cutting edge trends of polymer physics is mechanically induced chemiluminescence. Upon stress application, broken chemical bonds send out visible light. Thus, the intensity of the emitted light can be directly used to verify the underlying damage evolution in the polymer. In this contribution, a physically-based constitutive model capturing the mechanoluminescence in mechano-chemically responsive polymeric materials is proposed. Within the network model, the numerical integration over the unit sphere is avoided by using the analytical network-averaging concept [1]. The damage evolution is analytically computed in accordance with the principle of maximal dissipation. The

proposed model includes a few physically motivated material constants and demonstrates excellent agreement with multi-dimensional experimental data of dioxetane cross-linked filled elastomer. The result demonstrates a wide range of application of the analytical network-averaging concept.

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Modeling of PLLA near glass transition temperatures

S. Raza (Leuphana Universität Lüneburg), B. Klusemann (Leuphana Universität Lüneburg, Helmholtz-Zentrum Geesthacht) 15:40

The treatment for Coronary Heart Diseases - caused by the deposition of plaque on arterial walls - which has been the deployment of metal stent in the blocked artery, poses serious complications in the form of accumulation of blood clots due to the permanent and rigid nature of metals. Meanwhile, Bioresorbable Vascular Scaffolds (BVSs) - made up of poly l-lactide (PLLA) - are transient implants offering support to artery for 6-9 months and leaving no trace behind once dissolved after 2 years. PLLA, however, has lower strength compared to metals and thus requires a higher thickness to make it useful for transplants. Thermal annealing, which can alter the microstructure of PLLA to make it thinner and stronger, is a good solution for this problem. In order to implement thermal annealing, experimentation and simulations are required to study the behavior of the microstructure during the process. In general, its behavior below glass transition temperature and at short time-scale is glassy, while above glass transition temperature and at long time scale is rubbery. With constitutive models available for other polymers, such as polyethylene terephthalate (PET) - not only a significant polymer due to its extensive industrial use but also a polymer that is temperature and strain-rate sensitive - it is intended to develop a constitutive model for PLLA accordingly. In this regard, the well-known Buckley model is implemented and extended. The model allows to study the microstructural behaviour in PLLA at the temperatures of interest during thermal annealing. Numerical results will be presented and compared for neat PLLA samples for different strain rates and temperatures.

S 6a : Material modelling in solid mechanics

Thursday 16:30 - 18:30 Marienstr. 13, 1st floor, Lecture hall B

Chair: Martin Weber (Otto-v.-Guericke-Universität Magdeburg)
Lu Trong Khiem Nguyen (Universität Stuttgart)

Data-driven computational method for continuum mechanics within the finite strain theory

L. Nguyen (Universität Stuttgart), M. Keip (Universität Stuttgart) 16:30

The so-called data-driven computational method initiated by Kirchdoerfer and Oritz has been successfully applied to the linear elasticity problems. Basically, a complete continuum mechanics consists of three ingredients: the compatibility condition on the displacement field, the conservation laws, and the material laws that relate the strain and stress measures and are expressed as functional relationships between strains and stresses. Such relations have been proposed based on empirical observation data and thus are uncertain. In data-driven computational merit such functional relation is replaced with a collection of material data. The compatibility condition can be generally satisfied by employing the Galerkin or finite element method with proper use of basis functions and correct application of essential conditions. The conservation laws, or the principle of virtual work, can be approximated by a finite set of equations in a finite element procedure. These equations are regarded as equality constraints. Consequently, the data-driven problem can be expressed as an optimization problem: Find the point in the collection of material data points that minimizes the errors in the conservation laws and essential constraints. This work concerns the extension of the data-driven solver to the continuum mechanics in the finite strain regime. The corresponding optimization problem is stated for the material data in terms of the Green-Lagrange strain tensor and the second Piola-Kirchoff tensor. This choice of formulation leads to the symmetric or anti-symmetric tangent stiffness. Subsequently, the data-driven solver is tested on the truss systems, the continuum under plane stress and plane strain conditions with the material data being collected by perturbing the strain-stress curves of several existing material models.

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Modeling finite strain martensitic phase transformations in dual phase steels

J. Ruck (Karlsruher Institut für Technologie (KIT) - Institut für Technische Mechanik), T. Böhlke (Karlsruhe Institute of Technology (KIT)) 16:50

Modeling the transformation behavior of metallic materials due to thermal and mechanical loading is of great importance considering a variety of production processes and structural components. Prominent examples are high strength steels and shape memory alloys. Existing models describing the kinetics of phase transformations are either phenomenological models using empirical evolution equations, e.g. [1], [2], or

micro-
mechanical models. The micromechanical models are basically of two different kinds. First, there are laminate based approaches using relaxed potentials. The second group are sharp interface approaches modeling the transformation kinetics by considering an inclusion problem in a small strain framework [5].
The present work is concerned with the austenite martensite transformation behavior of the dual phase steel DP 600. To capture the transformation kinetics in terms of a sharp interface theory, a Rank-1 energy relaxation of the underlying free energy using laminates is applied, as proposed by [4]. To account for large transformation strains accompanied by large rotations a thermomechanical finite-strain framework is established. Numerical examples examining the effect of different load and temperature scenarios on the transformation kinetics are discussed. Furthermore a Finite-Element implementation using the UMAT interface of Abaqus is considered and numerical examples are discussed.

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Isogeometric Analysis of Second-Gradient Elasticity

R. Makvandi (Otto-von-Guericke University Magdeburg), D. Juhre (Otto-von-Guericke University Magdeburg) 17:10

The elastic energy in the conventional Cauchy continuum model depends on the gradients of the displacement field, which are not adequate to show the behavior of the system under point and line forces. Applying these kinds of boundary conditions to the continuum will lead to singularities. On the way to overcome this problem, generalization of the Cauchy continuum concept is inevitable.
Recently, Reiher et al. [1] presented a new concept for including second- and third-gradient material behaviors. Using the classical finite element method, they showed that in the presence of edge and tip displacements, in order to have a continuous solution for the displacement field, a second- and a third-gradient material is required, respectively. The presented partial differential equations were of order two (for second-gradient materials) and three (for third-gradient materials) which, respectively, need C^1 and C^2 continuity across the solution field. The classical finite elements (with mostly Lagrange

polynomials as shape functions) typically can only provide C^0 continuity, therefore they used Lagrange multipliers to overcome the need of higher-continuity elements by splitting the higher-order differential equation to multiple first-order equations. This, however, increases the computational costs drastically because of the need to introduce new degrees of freedom. The alternative method, is to use higher-order numerical methods such as Isogeometric Analysis (IGA).
Isogeometric Analysis is a generalization of the well-known finite element analysis (FEA) which has attracted attention of many researchers [2]. Introduced with the goal of capturing the gap between the computer aided design (CAD) and analysis software regarding geometry and meshing problems, IGA also provides a higher continuity comparing to the classical finite element thanks to using non-uniform rational basis splines (NURBS) as the analysis basis functions, which provides the ability to consider higher-order partial differential equations.
In this contribution, IGA will be used to simulate the behavior of second- and third-gradient materials. A development on an IGA-code has been done in order to add the calculation of global second- and third-derivatives of NURBS shape functions, hence no need to use Lagrange multipliers. A significant improve in the efficiency and accuracy of the attained results, comparing to the finite element results, is expected.

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On hyperelastic modeling of graphene based structures

R. Ghaffari, R. Sauer 17:30

In this paper, the hyperelastic membrane model of [1] for graphene is extended to a rotation-free shell formulation based on curvilinear coordinates and isogeometric finite elements [2, 3]. Exact quantum data are used to calibrate the model. This model is very close to experimental and full ab-initio simulations. Indentation and peeling of graphene and torsion and bending of carbon nanotubes are analyzed and the results are compared with atomistic data from the literature. The contact between substrate and graphene is modeled by the Lennard-Jones potential and the coarse grained contact model [4, 5].

Keywords: adhesive contact; carbon nanotubes; graphene; hyperelasticity; isogeometric finite elements; rotation-free shell.

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Thermodynamically Consistent Modelling of Recrystallization and Grain Coarsening in Precipitation-Hardened Alloys

L. Kertsch (Fraunhofer-Institut für Werkstoffmechanik IWM), D. Helm (Fraunhofer-Institut für Werkstoffmechanik IWM) 17:50

The strength of technically relevant alloys is mainly determined by the grain size distribution, the amount and size of precipitates, solid-solution hardening and work hardening. A reliable material model to capture these effects should be formulated within a comprehensive thermodynamic framework. The strategy of Rational Extended Thermodynamics is applied to derive a thermodynamically consistent model representing the coupling between elastoplastic deformation, the evolution of the grain structure and recrystallization. In addition, the model takes the dragging effect of precipitates on grain boundaries and dislocations into account, which leads to significant strengthening. For the microstructure description, a mean-field approach is used. Due to the thermodynamic framework, the model is able to consistently predict the interplay between deformation, microstructure evolution, dynamic hardening and softening and the related temperature change.

Material Plasticity to model the change of elastic anisotropy at finite strains

M. Weber (Otto-von-Guericke Universität Magdeburg), R. Glüge, A. Bertram (Otto-von-Guericke Universität Magdeburg) 18:10

We present a phenomenological finite elasto-plasticity theory which is capable to describe the evolution of the elastic anisotropy. The theory is called Material Plasticity after [1] and [2]. It is applicable to, e.g., fibre-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 this purpose we extend the known isomorphy concept (see [3]) using one second order tensor transforming the stress-free placement and a second transformation (also a second order tensor) which rules the evolution of the striffness tetrad.

We used a procedure which is able to determine the stiffness tetrad of the material before and after a large plastic deformation. Afterwards both stiffness tetrads are

compared. In this work we investigate uniaxial (effectively transversal isotropic symmetry), bidirectional (effectively tetragonal symmetry) and tridirectional (effectively cubic symmetry) reinforced material samples. We construct representative volume elements (periodic boundary conditions, see [4]) for the three samples. On the microscale we use an elastic-plastic material model for large deformations. After calculating the effective stiffnesses of the different material samples we investigate their evolution during different deformations. It turns out that it is possible to predict their evolution for the investigated materials with sufficient accuracy using one additional second order tensor. With this feature it goes beyond the usual multiplicative plasticity. After observing the change in the stiffness tetrads we finally introduce an analytical evolution equation for this tensor.

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S 6b : Material modelling in solid mechanics

Thursday 16:30 - 18:30 Marienstr. 13, 1st floor, Lecture hall D

Chair: Johanna Waimann (Ruhr-Universität Bochum)
Michele Marino (Leibniz Universität Hannover)

Biomaterial Spider Silk: Potential Candidate for Airbag Fabric Material

K. Prajapati (The Sirindhorn International Thai-German Graduate School of Enginnering), S. Patil (Institut für Allgemeine Mechanik), J. Carmai (The Sirindhorn International Thai-German Graduate School of Enginnering), S. Koetniyom (The Sirindhorn International Thai-German Graduate School of Enginnering), B. Markert (Institut für Allgemeine Mechanik) 16:30

Airbags are designed to protect occupants from fatality during an event of crash. During collisions, airbags are deployed within 20 to 30 milliseconds. In this time period, the airbags accelerate at very high rate, and the head of the occupants hits the airbag due to their own inertia. This causes various injuries like ocular trauma, contusions, neck

injury. Hence, airbags do save lives, but more research is needed on them to further reduce the injury severity of the driver and passenger. One of the most efficient ways to reduce injury risk is by transforming impact energy to permanent deformation. The larger the deformation, more energy is dissipated. Taking inspiration form a natural material is one of the most effective ways to develop a new material. Here, we propose spider silk material, which has extraordinary mechanical properties. The main goal of this work is to combine and simulate the mechanical properties of a spider silk web as an airbag and to study whether incorporating these material properties will be beneficial or not. To this end, we shall design an airbag with spider silk material properties, perform impact analyses and compare then with impact simulations of a standard airbag.

A stereologic approach for the spherical void size distribution in Polyurea

T. Reppel (Universität Siegen), K. Weinberg (Universität Siegen) 16:50

Polyurea is a high performance elastomer usually used as a protective coating on steel or concrete. Various elastic properties of Polyurea have been identified in the past, cf. [1], where in uniaxial tension a Young's modulus of about 65 MPa was measured together with an elongation up to 650%. After the long elastic range however, Polyurea fails like a porous material. This work aims at the approximation of the spherical void size distribution and it's influence on the material behavior, e.g. damaging effects.
To avoid the high costs for creating micro-CT images of Polyurea specimens, we use stereologic methods to estimate the size distribution of the spherical void radii. This is done with the usage of the classical Wicksell [2] approach by calculation the void section radii distribution from sliced specimens.
We consider several parametric and non-parametric distributions of the voids sections. With the use of Monte-Carlo simulation possible void radii distributions are obtained and verified in Wicksell's model. From the obtained distribution we deduce the influence of the voids on the damage behavior of Polyurea.

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Multi-scale modelling of fiber reinforced composites exhibiting elastoplastic deformation.

R. Bedzra (Institute of Applied Mechanics, RWTH Aachen University), J. Simon (Institute of Applied Mechanics, RWTH Aachen University), S. Reese (Institute of Applied Mechanics, RWTH Aachen University) 17:10

Composite materials are formed by a combination of two or more materials to achieve properties that are superior to those of its constituents. They consist mainly of unidirectional fibers or textile fabrics which are embedded in a matrix material. Depending on

the application, there are a variety of fiber/matrix combinations. Besides the anisotropic structure, the stress- strain response of these materials can be highly non-linear for fibers that behave elastoplastically.
Modelling such a material requires the consideration of different length scales in order to capture the intrinsic micro-structure of the composite material in the structure computation on the macro-level. To accomplish this, a finite element model of a repeating unit cell (RUC) of a unidirectional composite with tungsten fibers and copper matrix is set up. Virtual experiments are performed on the RUC by means of computational homogenization to identify the yield surface of the composite. Based on the obtained yield surface, a phenomenological material model which makes use of the concept of structural tensors is derived. This material model is then employed as the tows of a second generated RUC of a plain weave composite. Again, the yield surface of the plain weave composite is determined through virtual experiments and a second phenomenological material model is used to capture the response of the plain weave composite. The second material model then serves as the material of the composite on the structural level.
Keywords: Composite materials, Anisotropic plasticity, Repeating unit cell

Constitutive response and structure of soft biological tissues: direct and inverse identification of parameters

M. Marino (Leibniz Universität Hannover), M. Von Hoegen (Universität Duisburg-Essen), J. Schröder (Universität Duisburg-Essen), P. Wriggers (Leibniz Universität Hannover) 17:30

Soft biological tissues can be regarded as composite materials where families of collagen fibres are embedded in a ground matrix. Tissue constituents have a precise hierarchical and multiscale organization which confers highly nonlinear mechanical properties, characterized by finite-strain regimes and anisotropic fetures. The constitutive properties of tissues are generally described by introducing suitable expressions for the strain-energy function based on exponential or polynomial laws that involve invariant-based strain measures. Accordingly, the values of the parameters that are introduced in constitutive laws do not generally have an evident relationship with structural features.
The identification of the values of constitutive parameters is a main issue for developing reliable computational models of macroscale biological structures. The stress and strain patterns predicted by in silico approaches is indeed fundamental for analysing mechanobiological stimuli, interactions with prosthesis and devices, and failure response. Moreover, changes in the structural components of soft biological tissues, such as the properties of collagen fibres, have been shown to play a significant role in the pathogenesis of tissue degeneration. Computational models developed with the aim of analysing the response of pathological biological structures shall incorporate the structural differences of constitutive properties as otherwise simulations might not be good predictors for the actual in vivo stress and strain state.
The aim of this work is to find the correlation between the parameters of classical macroscopic strain-energy functions, based on a phenomenological description of colla-

gen nonlinearities, with collagen-related tissue properties. Both microscale histological features and nanoscale biochemical characteristics are addressed, focusing on collagen arrangement, fiber radius and amplitude, as well as intermolecular cross-link density and molecular persistence length. By following a direct approach (from structure to model), parameter identification is based on an optimization problem, choosing as reference the constitutive response obtained from a multiscale homogenization technique which incorporates mechanisms occurring from the nanoscale (i.e., collagen triple helix), through the mesoscale (i.e., cross-linked molecular assemblies), up to the microscale (i.e., crimped fibers). The obtained direct structure-parameters relationship is based on a numerical procedure, which is then generalized by introducing a closed-form relationship by means of a nonlinear regression analysis. Results are also presented for the inverse estimation of structural features from mechanical parameters, opening to the development of novel approaches for gaining histological and biochemical information that could be employed both in diagnosis and therapy.

On the modelling of curvature effects in fibre-reinforced nanocomposites

T. Asmanoglo (Institute of Mechanics, TU Dortmund), A. Menzel (Institute of Mechanics, TU Dortmund and Division of Solid Mechanics, Lund University) 17:50

Motivated by experimental findings on one-dimensional nano-materials, we elaborate a specific form of the stored energy function which takes into account higher-order gradients of the placement field in terms of the fibre-curvature. Thus, making use of an extended continuum approach a natural length scale is introduced into the model which allows us to account for the experimentally observed size effects. The utilized framework is based on theoretical developments on fibre-reinforced composites (presented in Finite deformations of fibre-reinforced elastic solids with fibre bending stiffness, International Journal of Non-Linear Mechanics, 42(2):355-368, 2007), which focus on the extension of the classical structural tensor based modelling approach by assuming that the fibres resist bending. This approach results into a coupled system of non-linear partial differential equations which we propose to solve by making use of a mixed-type multi-field finite element scheme.

Finite element implementation and simulation of the functional fatigue in shape memory alloys

J. Waimann (Institute of Mechanics of Materials, Ruhr-Universität Bochum), P. Junker (Institute of Continuum Mechanics, Ruhr-Universität Bochum), K. Hackl (Institute of Mechanics of Materials, Ruhr-Universität Bochum) 18:10

Due to the effects of pseudoelasticity and pseudoplasticity, shape memory alloys are very promising materials whose industrial usage has lagged behind its potential. The reason for that is the functional degradation during cyclic loading - more precisely the effect of functional fatigue which occurs during pseudoelastic loading. The effect is modeled by subdividing the diffusionless solid/solid phase transformation into a reversible and

an irreversible process which is an experimentally motivated ansatz for the modeling of the complex material behavior. Thus, we will take into account a reversible and an irreversible volume fraction for the austenitic and several martensitic phases. To consider the material's polycrystalline structure and thus differently oriented grains, we will use an orientation distribution function which depends on three Euler angles and affects a high numerical efficiency as presented in [1].

First of all, we will present a fast and phenomenology-free material model which is easy to calibrate and based on variational principles, more precisely the principle of the minimum of the dissipation potential. Furthermore, the focus of our presentation will be the finite element implementation and simulation of the complex material behavior. We will prove our material model's functionality by various calculation results which are of mesh-independent character, see also [2].

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S 6a : Material modelling in solid mechanics

Friday 09:00 - 11:00 Marienstr. 13, 1st floor, Lecture hall B

Chair: Abbas Tutcuoglu (California Institute of Technolog)
Hossein Talebi (Helmholtz-Zentrum Geesthacht)

Thermomechanical Simulation of Friction Stir Welding of Aluminum 2024 Using an Adaptive Element-Free Galerkin Method

H. Talebi (Helmholtz-Zentrum Geesthacht), M. Frönd, J. Dos Santos, B. Klusemann (Leuphana University of Lüneburg, Helmholtz Zentrum Geesthacht) 09:00

The coupled themomechanical modeling of the friction stir welding (FSW) process is a challenging process when typical finite element methods are used. In this study we use a meshfree technique to model the material flow during the FSW process. We employ the Element Free Galerkin Method (EFG) as approximation method. A mortar contact is used to account for the stirring effect and heat generation from the frictional contact. We use a two-way adaptive method (rh-adaptive) during the coupled thermomechanical process to overcome potential numerical problems arising from the extensive mesh distortion and material deformation. This means, the mesh is globally refined with perusing an anisotropic tetrahedral mesh (h-adaptive). At the same time,

a completely new mesh is built based on the old mesh (r-adaptive). Finally, we validate our simulation results with comparison to experiments done on 6mm thick Aluminum (AA2024-T351) sheets with a Triflat conical threaded tool. The comparison of the numerical results and experiments show good agreement. The next step after this study is to use the deformation and temperature history from the thermomechanical simulation to predict the final micro-structure after the welding process where the dynamic recrystallization is responsible for the micro-structure evolution.

Thermomechanically coupled crystal plasticity modeling of fully lamellar TiAl with emphasis on Hall-Petch effects

J. Schnabel (Helmholtz-Zentrum Geesthacht), S. Bargmann (University of Wuppertal) 09:20

Fully lamellar TiAl alloys are increasingly used as structural materials for high temperature applications e.g. for turbine blades in low-pressure stages of aircraft engines. These structurally demanding applications necessitate precise knowledge of the materials thermomechanical behavior to ensure safe operation.
The numerous microstructural interfaces in fully lamellar TiAl alloys give rise to three concurrently acting Hall-Petch effects which collectively induce their high strength. So far, their relative contributions could not be separated uniquely in experiments.
The thermomechanically coupled crystal plasticity model, presented in this contribution, enables to overcome this experimental limitations and helps to separately quantify the three different Hall-Petch effects using literature experimental results. This micromechanical model reflects the morphology of the lamellar compound in a single colony, i.e. on micro scale, and captures its complicated hardening behavior up to 10% plastic strain. Subsequently, this micro scale model is transferred to a meso scale polycolony RVE in order to get insight into the complex interrelations between the different microstructural strengthening effects.
The model nicely captures the micro yield and micro hardening in fully lamellar microstructures and the extracted Hall-Petch slopes help to explain the spread in reported experimentally determined values.

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Virtual testing of sheet metals: Predicting mechanical properties from microstructure simulations

J. Pagenkopf (Fraunhofer Institute for Mechanics of Materials IWM), A. Butz (Fraunhofer Institute for Mechanics of Materials IWM), M. Baiker (Fraunhofer Institute for Mechanics of Materials IWM), D. Helm (Fraunhofer Institute for Mechanics of Materials IWM) 09:40

Due to the crystallographic texture that is a result of processing steps like rolling and annealing, sheet metals often have anisotropic mechanical properties. For the simulation of sheet metal forming processes it is important to incorporate an accurate description of the material behavior by using suitable anisotropic yield functions.
In this contribution, we apply a numerical homogenization scheme based on full-field finite element simulations and a crystal plasticity material model to predict mechanical properties for different sheet-metals. Using this approach, we show how anisotropic yield functions (e.g. Hill48, Yld89, Yld2000-2d), that are widely used in industrial applications, can be calibrated for single-phase sheet metals. The virtual testing framework has several advantages: (1) The simulation results extend the experimental data that are required for the identification of model parameters. Thus, the identification procedure can be improved and the experimental effort may be reduced. (2) Since it is possible to generate a great number of points on the yield surface, more complex models with many model parameters (e.g. BBC2008) can be calibrated. (3) The approach helps to study structure-property relations of the material and can be applied in material design processes.
However, the results of the strategy depend on the quality of the microstructure representation in the simulations. Using dual-phase steels as an example, we show how the level of detail regarding the representation of microstructural features (like the crystallographic texture and the martensite morphology) affects the accuracy of the predicted mechanical properties by comparing the simulation results with experimental data.

NUMERICAL MODELING OF DYNAMIC RECRYSTALLIZATION IN POLYCRYSTALS

H. Nguyen (Ruhr-Universität Bochum), V. Ebrahimzade, B. Trinh, J. Renner, K. Hackl (Institute of Mechanics of Materials, Ruhr-Universität Bochum) 10:00

This paper is devoted to developing a mathematical model of dynamic recrystallization phenomena based on the earlier work of K. Hackl and J. Renner [1] for polycrystalline materials. In this model a variational approach employing a distribution function for dynamic recrystallization processes of polycrystalline materials is presented. It is based on a marching algorithm at the microscale as well as a homogenization procedure to arrive at the macroscale. The newly proposed theory is now used to improve the variational approach. Then this theory is applied within the homogenization procedure. A comparison of the present model with existing phenomenological ones is given.

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A finite plasticity model with a smooth elastic-plastic transition

M. Jabareen (Technion - Israel Institute of Technology) 10:20

Generally speaking, constitutive equations for elastic-plastic materials are formulated in terms of a yield function and evolution equations for the rate of plastic deformation and

hardening variables. These constitutive equations can be developed by using number of approaches with different classes of kinematic decomposition (e.g. additive split of the Lagrange strain, multiplicative split of the deformation gradient, additive split of the rate of deformation, etc.). However, in these formulations the consistency condition, which causes the yield function to vanish during loading, also causes the transition from elastic to plastic response to be sharp with a distinct break in the slope of the stress-strain curves. In the present work, a general theoretical framework for modeling a smooth elastic inelastic transition for large deformations of rate independent elastic-plastic and rate dependent elastic-viscoplastic materials has been proposed.
A special finite element formulation was developed for the general plasticity model, in which the reference configuration of the body is treated as an initial condition, and the formulation depends only on two consecutive configurations. A number of example problems for large deformation have been considered which examine and verify the implementation of the developed finite element, and in particular show that the integration scheme for the elastic distortional deformation is strongly objective.

Computational modelling of texture evolution in HCP metals under finite deformations

A. Tutcuoglu (California Institute of Technology), V. Ananthan (California Institute of Technology), K. Bhattacharya (California Institute of Technology), Y. Chang (The MathWorks, Inc.), D. Kochmann (California Institute of Technology) 10:40

Optimal grain size control through processes such as equal channel angular pressing (ECAP) are of central importance in the tailoring of macroscopic material properties, including specific strength and creep performance. Numerous models provide the means to simulate the two major mechanisms underlying microstructure evolution under plastic deformation, namely, texture evolution and recrystallization, but are generally confined to small strains or face-centered cubic (fcc) metals. However, both the presence of twinning in hexagonal close-packed (hcp) metals as well as the inherently large deformations in ECAP demand for new alternatives. The model we present affords the solution to the microscopic initial boundary value problem (IBVP) for a representative volume element (RVE) based on the Fast Fourier Transform (FFT). The time evolution of internal variables throughout the RVE is performed on the basis of a variational constitutive model for slip-twinning interactions in finite deformation kinematics. We apply the model to simulate texture evolution in pure Mg during severe plastic deformation. In the framework of finite deformations, non-uniqueness problems in grain boundary migration caused by the absence of a unified rotation throughout a grain are met by imposing additional crystallographic constraints. The results are compared to a computationally inexpensive Taylor model.

S 6b : Material modelling in solid mechanics

Friday 09:00 - 11:00 Marienstr. 13, 1st floor, Lecture hall D
Chair: Alexander Lion (Universität der Bundeswehr München)

From discrete 3D to 2D and analytic models of electrospun fibre mats

S. Domaschke (EMPA), M. Zündel (ETH Zürich), E. Mazza (ETH Zürich), A. Ehret (EMPA) 09:00

Electrospun nanofibre networks have growing use in technical and biomedical applications, e.g. for filters, or scaffolds in tissue engineering applications. Computational analyses and predictive simulations of these materials require suitable mechanical models to describe their behaviour. Generally, such models can be based on either representative volume elements in three or two dimensions by discretizing the single fibres in terms of finite elements, or on continuum models representing the homogenized response of the network. While 3D discrete fibre models are able to account for the spatial orientation of fibres and their interaction through crosslinks and the temporary contacts forming during the non-affine deformation of the fibres, particularly the latter entail high computational cost. Since in the thin electrospun mats, the interaction between fibres through the thickness is typically limited, a simplified 2D, i.e. planar representation of the network provides an efficient alternative. In the present contribution, we present methods to create 2D and 3D representative volume elements of discrete network models specific for electrospun materials by "virtual spinning". These methods are used to generate corresponding 2D and 3D networks, i.e. with similar segment length and fibre orientation distribution, as well as comparable fibre intersection density. Assuming the same single fibre behaviour for both networks, their performance is compared in terms of their macroscopic responses and computational effort. Finally, the discrete network models are utilized to investigate typical assumptions used by analytical modelling approaches for electrospun networks.

Analysis of Gold Micro-Beams with Higher Order Continuum Theories

M. Kandaz (Middle East Technical University), H. Dal (Middle East Technical University), M. Unlu (Yildirim Beyazit University) 09:20

Microbeams are building blocks for many micro and nanostructures as well as microelectromechanical systems (MEMS) and cannot accurately be modelled by classical continuum theories due to size effects due to their micro-scale. These size effects can be taken into account by the so-called higher order continuum theories. *Modified Strain Gradient Theory* (MSGT) and *Modified Couple Stress Theory* (MCST) are two commonly used theories, which extend the classical local continuum theories of grade one with the introduction of additional length scale parameters. In this contribution, the variational problem governing the elasticity of higher order beam formulation and the finite element implementation based upon, are briefly introduced. To this end, well known Euler-Bernoulli beam formulation assumptions are used. The size effect for

gold-micro beams is demonstrated and the length scale parameters of gold micro-beams for MSGT and MCST are identified form the existing experimental data from literature for the first time. As a novel aspect, significant size effect is demonstrated for the length scales associated with the state of the art gold micro-beam structures developed for NEMS and MEMS applications, which reveals the necessity of the use of higher order theories at these length scales. Advantages and drawbacks of these theories are also discussed comparatively.
Keywords: gold microbeams, higher order continuum theories, modified strain gradient theory, modified couple stress theory, length scale parameters, finite element analysis, size effects

Space-time data compression for nonlinear viscoelastic systems in cyclic processes

M. Hassani (EMMA- Efficient Methods for Mechanical Analysis, University of Stuttgart), F. Fritzen (Universität Stuttgart) 09:40

The inherent large-scale complexity of nonlinear models leads to unmanageable levels of storage and computational requirements. One approach for overcoming this is through Model Order Reduction (MOR). Model reduction aims to reduce this computational burden by generating reduced models that are faster and cheaper to simulate, yet accurately represents the original large-scale system behavior. An example of MOR for application in nonlinear homogenization is the potential based reduced basis model order reduction (pRBMOR) [1], which can be used to solve numerical multiscale problems on desktop computers [2].

For space-time model reduction, we are interested in applying pRBMOR to structural problems subjected to long-term loading in the presence of nonlinearities by extending it to operate in space-time. In order to achieve this goal a non-standard discretization approach is considered, in which beside the classical FE discretization, the internal degrees of freedom are considered as additional unknowns. The obtained RB represents the behavior in a complete time period, e.g. one load cycle. Thus we project the reduced stationary conditions on the time domain. Investigations regarding the identification of the reduced space-time basis for nonlinear visco-elastic materials subjected to sinusoidal loading are presented. Furthermore, the capabilities of our model in case of long-term loading are shown for creep test.

Refrences

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Experimental and Micro-Macro Integrated FE Investigation of Texture and Microstructure Evolution in Polycrystalline Ag-SnO2 Metal Matrix Composites

Y. Schneider (Institute for Materials Testing, Materials Science and Strength of Materials (IMWF)), W. Wasserbaech (Institute for material science (IMW)), S. Schmauder (institute for materials testing, materials science and strength of materials) 10:00

In order to be environmentally friendly, it requires that the industrial products possess properties being suitable for the physical loadings and for the health. The Ag-SnO2 metal matrix composite is one of such materials and widely applied for electrical contacts in the automobile industry. Before in service and after the manufacture process, usually, one performs the tensile hot extrusion load on it more than one time. In the current work, we take polycrystalline Ag-17vol.%SnO2 as a sample material produced by powder metallurgy and put the emphasis on investigating its microstructure and texture evolution. Experimentally, the stress-strain behaviour, the macro and micro texture evolution, the misorientation and hardness, are studied for both the monotonic tensile and the hot extrusion loading. Numerically and for the first step, the micro-macro integrated finite element (FE) simulation is aimed to predict the tensile behaviours, like, the stress-strain relationship, the microstructure and texture evolutions, as aforementioned in the experiment. For the sake of simplicity and considering to apply the real microstructure obtained from EBSD measurements, we prefer the axisymmetric analysis in ABAQUS. Since the deviation of the particle volume fraction in FE may be large compared to the real one, a numerical method will be presented to position the microstructure cut-out in the macrostructure aimed to minimize the above mentioned mismatch. Microscopically, the Ag polycrystals are simulated by the elasto-visco-plastic material model, where the particle phase SnO2 is assumed to be elastically deformable. The hardening of the composite behaves isotropically for the macrostructure in FE.

Modelling the thermoplastic material behaviour of a tailored formed joining zone on a microscopic length scale with focus on the steel component

M. Baldrich (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), S. Löhnert (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 10:20

Tailored Forming is a technology in which two different metallic materials are joined before being formed together. This has the advantage of possible weight reduction of the engineering part and optimized material distribution with regard to the applied loads. One weakness of the technique however is the joining zone which due to the significant differences of the stiffnesses of the joined materials may suffer from high stresses during the forming process that might lead to damage and failure. As a result, it is important to accurately predict the material behaviour of the joining zone. For this reason a physically motivated material model needs to be developed so that the thermomechanical properties of the joining zone during and after the tailored forming

process are represented.
Because of the strong dependence of the effective, macroscopic material behaviour on the thermomechanical and chemical influences on the microscopic level, the polycrystalline material is investigated on the microscopic length scale. Therefor, on the one hand the morphology of the joining zone and on the other hand the material behaviour of the different components, ferrite, pearlite and aluminium, are considered in detail. The approach for the geometric model generates non-convex grains of variable sizes with different orientations of the atomic lattice according to /1/. Based on /2/ the microscopic material behaviour of the different components of the joining zone is described considering the atomic lattice and its orientation, the slip systems and dislocation densities as well as the critical stresses and deformation rates.
In a future step, due to the occuring diffusion caused by heat treatment and mechanical pressure, the material model will be extended to reflect the strongly coupled thermo-chemo-mechanical behaviour by adding a diffusion term for the material concentrations. Then, it will be possible to capture the changes of concentration of the different components in the joining zone and the emerging modification of its properties. Finally, to obtain the material behaviour on a macroscopic length scale, the micromechanical material model will be homogenized and embedded in a specialized macroscopic cohesive zone element.

/1/ Beese, S., Löhnert, S., Wriggers, P.: Crack Propagation in poly crystalline materials, ECCOMAS, X-DMS, 2015, sciencesconf.org:x-dms2015:64199
/2/ Zeller, S., Löhnert, S. and Wriggers, P. (2015), Modelling thermoplastic material behaviour of dual-phase steels on a microscopic length scale. Proc. Appl. Math. Mech., 15: 373–374. doi:10.1002/pamm.201510177

An explanation of damage and failure in polysaccharidic aerogels: model approach

A. Rege (Department of Continuum Mechanics, RWTH Aachen University), M. Itskov (Department of Continuum Mechanics, RWTH Aachen University) 10:40

Cellulose aerogels can be considered as foam-like materials and have recently been modeled using a micro-mechanical approach [1]. The proposed square cell network model is based on the bending of the cell wall fibrils and shows good agreement with experimental data under moderate strains. Under compression, the cell walls undergoing bending start to buckle upon reaching a critical buckling load [2-4]. On the other hand, under tension the deformation in the cell walls is stretching dominated [3]. Accordingly, the total aerogel network energy is divided into a bending one and a tension one. The cell walls undergoing buckling/stretching further collapse/fail after reaching a critical stretch value, and are then considered to no longer contribute to the total network energy. The model parameters are either obtained from experimental observations, like the pore-size data analysis, or from molecular dynamics simulations, thus resulting into a physically

motivated model. Finally, the model is also shown to be effective in predicting the constitutive response of other polysaccharidic aerogels.
[1] A. Rege, M. Schestakow, I. Karadagli, L. Ratke, and M. Itskov, Soft Matter 12, 7079 (2016)
[2] L. J. Gibson, J Biomech 38, 377 (2005)
[3] P. R. Onck, T. Koeman, T. van Dillen, and E. van der Giessen, Phys. Rev. Lett. 95, 178102 (2005)
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S 6a : Material modelling in solid mechanics

Friday 11:30 - 13:30 Marienstr. 13, 1st floor, Lecture hall B
Chair: Wolfgang Weber (TU Dresden)
Christian Woitzik (Hamburg University of Technology)

Ideas regarding a physically motivated selection of snapshots for POD calculations – application to z-pin pullout

W. Weber (Technische Universität Dresden, Institute of Mechanics and Shell Structures), Y. Fangye (Technische Universität Dresden, Institute of Mechanics and Shell Structures), B. Zastrau (Technische Universität Dresden, Institute of Mechanics and Shell Structures), D. Balzani (Dresden Center for Computational Materials Science (DCMS)) 11:30

For the solution of typically large systems of equations resulting from nonlinear engineering problems, efficient numerical procedures are sought. One possibility to reduce the computational effort and simulation time is the use of model reduction methods, see e.g. the foreword of a special issue of MCMDS [2]. Within this contribution the method of choice is the proper orthogonal decomposition (POD), which is a powerful projection based reduction method with application in both linear and nonlinear solid mechanics [1, 3]. For applying the POD a reasonable number of snapshots is necessary. Herein, these snapshots are the results of FE analyses for given load regimes and time instances of the aforementioned problem. The question arises whether a science-based choice of these snapshots allows for taking a low number of snapshots into account within the POD. Hereto, a link to the eigenforms of the underlying mechanical system may be advantageous. Thus, relations between the proper orthogonal modes and the eigenvectors are revealed and discussed. The POD then is applied to the modeling of the z-pin pullout. Herein, z-pins are an innovative reinforcing of composites and are directed perpendicular to the middle-surface of thin walled structures in order to prevent these structures from delamination [4]. From such a structure, a representative material clip is investigated with respect to the pullout of a z-pin. The proper orthogonal modes extracted from the calculated data of the FE analyses of the pullout are compared to the evolution of the tip displacement of the z-pin which stems from a simplified analytical

model describing this pullout.
[1] F. Bamer, C. Bucher. Application of the proper orthogonal decomposition for linear and nonlinear structures under transient excitations. Acta Mechanica 223 (2012), 2549-2563
[2] B. Lohmann, P. C. Müller. Editorial. Mathematical and Computer Modelling of Dynamical Systems 14 (2008), 389-390
[3] A. Radermacher, S. Reese. A comparison of projection-based model reduction concepts in the context of nonlinear biomechanics. Archive of Applied Mechanics 83 (2013), 1193-1213
[4] F. Warzok, G. Allegri, M. Gude, S.R. Hallett. Experimental characterisation of fatigue damage in single Z-pins. Composites: Part A, to appear

Laser shock peening process modeling and experimental validation for AA2198-T3 and AA2198-T8

S. Keller, N. Kashaev (Helmholtz-Zentrum Geesthacht), B. Klusemann (Leuphana University of Lüneburg, Helmholtz Zentrum Geesthacht) 11:50

Laser shock peening (LSP) is a surface treatment which improves the fatigue performance of metallic structures by inducing compressive residual stresses. A pulsed laser vaporizes the first layer of the component and turns the solid material into plasma. Thermal expansion of the plasma initiates high pressure shock waves within the material. Residual stresses are the result of local plastic deformations caused by the pressure waves. The process is highly nonlinear and difficult to optimize based on experiments alone due to the high number of process parameters and short time events which are hard to measure (e.g. shock wave propagation, plasma forming). Especially, the shock wave reflection at the back side of the specimen could influence the residual stresses and, therefore, extend the simulated time. The material under investigation is AA2198 at different temper stages, which shows a very pronounced rolling texture. AA2198 is an aluminum-lithium-alloy of the third generation and finds application in light weight structures (e.g. aircraft). Aiming to an deeper understanding of the process and an optimized residual stress profile, a finite element model is set up. A phenomenological Johnson-Cook material model is employed to predict the strain hardening and strain rate behavior. The work is split into two parts; at first, experiments are used to determine the requirements for the simulation. Experiments clarify the influence of the base layer and the influence of the initial residual stresses depending on the thickness of the specimens as well as the aspect of the material anisotropy. The laser is characterized by 5 J laser pulses with a squared focus of 3mm $\times$ 3mm or 1mm $\times$ 1mm. Residual stresses were measured by the incremental hole drilling method using electronic speckle pattern interferometry (ESPI). Secondly, a finite element model is employed enabling the identification of the laser induced pressure pulse for AA2198-T3. Laser pulse impacts were simulated with pressure boundary conditions, hence, the influence of the phase transition of the first material layer is neglected. The validity of the model will be shown for a LSP process simulation of AA2198-T8. Simulation and experimental measured residual stress profiles are for both temper stages in excellent agreement. Details about the employed numerical

scheme will be presented.

Finite element modeling of laser beam welding for residual stress

J. Herrnring (Helmholtz-Zentrum Geesthacht), N. Kashaev (Helmholtz-Zentrum Geesthacht), B. Klusemann (Leuphana University of Lüneburg, Helmholtz Zentrum Geesthacht) 12:10

Laser beam welding is a widely used joining process in industrial application. Within the process a highly inhomogeneous temperature field in the joined materials is generated, which causes changes in mechanical properties, residual stresses and component distortion. The high temperatures in the liquid pool and in the heat-affected zone lead to a severe change in material microstructure. The mechanical properties depend strongly on the microstructure and change therefore dramatically in the fusion- and heat-affected zone compared to the properties in the base material.
This work determines the residual stress field in a butt joined, precipitation hardened aluminum alloy via a phenomenological continuum model. The material behavior is defined by a thermomechanical material model, which changes the behavior from viscoplastic below the solidus temperature to a pure viscous behavior above the liquidus temperature. A mixed finite element formulation is used to ensure incompressible material behavior above the melting temperature. The temperature field is described based on the heat conduction equation in combination with a three-dimensional Gaussian power distribution. The temperature field is solved by a semi analytical solution which utilizes the method of Greens- Functions. As a consequence of the severe change of mechanical properties based on the dissolution of precipitations a kinetic model is used, which describes the dissolution of precipitations. Residual stresses of butt welded specimens are measured with synchrotron x-rays and compared with the numerically determined stress fields.

Prevention of solidification cracking during pulsed laser beam welding

M. Bielenin, J. Bergmann, J. Hildebrand, K. Schricker, R. Herzog, I. Riedel, C. Trunk, K. Worthmann 12:30

We present a mathematical model to describe laser beam welding based on the heat equation. Since the material coefficients depend on the temperature, this leads to a quasi-linear parabolic partial differential equation. It is our goal to prevent solidification cracking. We address this problem by means of optimal control. Here, the intensity profile of the laser beam acts as a control. The main challenge is the formulation of a suitable objective function. In particular, non-standard terms are used to penalize high velocity of the solidification interface in order to deal with cracking phenomena.

Statistical characterization of granular material applied as crash absorber in ship building

C. Woitzik (Hamburg University of Technology, 21073 Hamburg, Germany), M. Chaudry (Leibniz University Hannover, 30167 Hannover, Germany), P. Wriggers (Leibniz University Hannover, 30167 Hannover, Germany), A. Düster (Hamburg University of Technology, 21073 Hamburg, Germany) 12:50

Using modern simulation techniques it is possible to examine new application fields for granular materials. In ship building the collision safety is one of the main concerns. A widely used design concept are double hull ships, which consist of an outer and an inner hull with some void space in between. Filling up this void space with a granular material was suggested in [1]. The main reason for doing so consists of two aspects. On the one hand an improvement of penetration resistance due to a load transfer from the outer to the inner hull can be obtained. On the other hand an energy dissipation due to the crushing of granulate particles also helps to improve the collision safety. With modern simulation techniques these effects can be modelled and investigated in more detail using a coupled approach of the Discrete Element Method (DEM) and the Finite Element Method (FEM). To this end, the material parameters of the granulate have to be determined. A simplified approach for determining macroscopic material parameters of the granulate for the FEM was presented in [1, 2]. Here we consider the material parameters of single particles for the DEM.

Based on a list of requirements and uniaxial pre-tests of granules [2], expanded glass and expanded clay materials seem to be very promising. These lightweight granules have a diameter between 2 mm and 10 mm and a density below $400\,\mathrm{kg/m^3}$. Using these particles in a discrete element simulation, several material parameters are required, especially Young's modulus and the crushing strength [3]. Thus a uniaxial single particle compression test has been used to determine these parameters. Due to the manufacturing process and the general behaviour of single grains, the obtained parameters vary a lot. To overcome this uncertainty we divide each granulate into several fractions and develop a statistical model for its representation.

To model the distribution of Young's modulus and the crushing strength a logistic function is used. Compared to Weibull or log-normal distributions it stands out due to its simplicity. Different fractions are modelled with a diameter dependent function of the crushing strength and Young's modulus, respectively [4]. These diameter dependent models are combined with the diameter distribution of the granulate. In this way we obtain a two-dimensional model consisting of five or six constant parameters for the crushing strength-diameter distribution and the Young's modulus-diameter distribution, respectively. This approach can be extended to a simplified three-dimensional distribution, which covers all parameters of interest for one granulate with nine parameters. Using a numerical method for an inverse transformation, we can generate sample points and use these as input variables for a simulation based on the DEM.

[1] M. Schöttelndreyer (2015), Füllstoffe in der Konstruktion: Ein Konzept zur Verstärkung von Schiffsseitenhüllen. Techn. Univ. Hamburg-Harburg, Institut für

Konstruktion und Festigkeit von Schiffen, PhD thesis, Hamburg-Harburg, 2015. doi:10.15480/882.1258

[2] C. Woitzik, M. A. Chaudry, P. Wriggers, and A. Düster (2016), Experimental and numerical investigation of granular materials for an increase of the collision safety of double-hull vessels. Proc. Appl. Math. Mech., 16: 409–410. doi:10.1002/pamm.201610193

[3] M. A. Chaudry, C. Woitzik, A. Düster, and P. Wriggers (2016), DEM-FEM coupled numerical investigation of granular materials to increase crashworthiness of double-hull vessels. Proc. Appl. Math. Mech., 16: 311–312. doi:10.1002/pamm.201610144

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Numerical simulation of granular materials during confined compression

M. Chaudry (Leibniz Universität Hannover, 30167 Hannover, Germany), C. Woitzik (Hamburg University of Technology, 21073 Hamburg, Germany), A. Düster (Hamburg University of Technology, 21073 Hamburg, Germany), P. Wriggers (Leibniz Universität Hannover, 30167 Hannover, Germany) 13:10

Granular materials have applications in a variety of fields which includes among others metallurgy, civil engineering, food industry and pharmacy. Recently, it has been proposed that these materials can be used to increase the crashworthiness of double hull ships [1]. However, usage of such materials requires better understanding of their mechanical properties under different loading conditions. In this contribution, the behaviour of granular materials during confined loading is studied.

During confinement these materials are susceptible to crushing, where compressive loads exceeds the strength of the material. Numerical simulation of such complex phenomenon can be performed at the continuum level where the material response is computed via a macroscopic constituitive equation [2] or with the Discrete Element Method (DEM) where the analysis is carried out at the micro-mechanical level [3]. Here, for numerical simulation, a DEM framework based on the work of Wellmann [4] is employed. In DEM grains, referred here as particles, are treated as rigid bodies which have translational and rotational degrees of freedom assigned to their center of mass. For calculation of contact forces between particles the Hertz-Mindlin theory is applied whereas an explicit time integration scheme is used to update the position of the particles.

Compression tests provide ample insight into the mechanical behaviour of granular materials. This is investigated through numerical simulation of oedometric test. During such tests granular materials are subjected to a high confining pressure. Depending on the critical strength of the particles, extensive comminution is observed. Furthermore, in the framework of the DEM, computational aspects of comminution in such tests will also be discussed.

[1] M. Schöttelndreyer. Füllstoffe in der Konstruktion ein Konzept zur Verstärkung von Schiffsseitenhüllen. *Techn. Univ. Hamburg-Harburg, Institut für Konstruktion und Festigkeit von Schiffen, PhD thesis Hamburg-Harburg, 2015.*

[2] C. Woitzik, M. A. Chaudry, P. Wriggers, and A. Düster (2016) Experimental and numerical investigation of granular materials for an increase of the collision safety of double-hull vessels. Proc. Appl. Math. Mech., 16: 409 -410. doi:10.1002/pamm.201610193

[3] M. A. Chaudry, C. Woitzik, A. Düster, and P. Wriggers (2016) DEM-FEM coupled numerical investigation of granular materials to increase crash- worthiness of double-hull vessels. Proc. Appl. Math. Mech., 16: 311-312. doi:10.1002/pamm.201610144

[4] C.Wellmann, A Two-Scale Model of Granular Materials Using a Coupled DE-FE Approach. *PhD Thesis, Leibniz University Hannover* 2011.

S 6b : Material modelling in solid mechanics

Friday 11:30 - 13:30 Marienstr. 13, 1st floor, Lecture hall D
Chair: Alexander Lion (Universität der Bundeswehr München)

On the Modeling of Textile Membranes with Nonlinear Anisotropic Material Behavior

M. Motevalli, D. Balzani (Dresden Center for Computational Materials Science (DCMS)) 11:30

Coated tensile fabric membranes are thin structural elements which are utilized in civil engineering for the construction of e.g. facades and roofs. Due to their woven fabrication they are remarkably stiff under tension in in-plane directions and almost not resistant to bending loads. The mathematical description used in engineering practice nowadays for textile membrane materials is based on orthotropic linear-elastic formulations [3], where a specific behavior in the warp and fill directions is considered. However, these simplifications are not sufficient since a significant nonlinear behavior is observed in experiments, cf. [5]. Furthermore, a pronounced lateral contraction is found, which can not be represented by a linear elastic model since the associated tangent matrix is not positive definite and thus not applicable in numerical simulations.
In this contribution we focus on the construction of a suitable anisotropic polyconvex energy function in the geometrically nonlinear setting. In order to capture the anisotropic behavior, we make use of structural tensors and formulate the strain energy as a function of principal and mixed invariants of the right Cauchy-Green and the structural tensors. By choosing a polyconvex strain energy function we assure the existence of minimizers and Legendre-Hadamard ellipticity [1], [2] and [4]. We adjust the parameters such that the model response is as similar as possible to the experimental data by minimizing an

objective function. The basis is stress-strain data in two uniaxial tension tests in the warp and fill direction. In these experiments we prescribe the axial force and measure the deformation in axial-, lateral- and thickness direction. As it turns out, by increasing axial deformations, negative lateral strains and positive thickness strains are obtained, owing to the wavy structure of the textile fabric. The objective function is therefore formulated such that the 1st Piola-Kirchhoff stress and the lateral and thickness deformation gradient of the model response is compared with the experimental quantities. For the model response, the axial (measured) deformation gradient is prescribed and the lateral and thickness stress is iterated to zero.

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[2] D. Balzani, P. Neff, J. Schröder, G.A. Holzapfel, A Polyconvex Framework for Soft Biological Tissues. Adjustment to Experimental Data, Int. J. Sol. Struct. 43, 6052-6070 (2006)

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Distribution of dislocations in twisted bar

K. Le (Ruhr Universität Bochum/ Lehrstuhl für Mechanik - Materialtheorie), Y. Piao (Ruhr Universität Bochum/ Lehrstuhl für Mechanik - Materialtheorie) 11:50

In our task, it proposes an asymptotically exact continuum dislocation theory (CDT) of single crystal bars under torsion, in which we assume there only exists screw dislocations and they will be treated as a point singularity on the bar‘s cross section, where dislocations are parallel to the bar axis. Under non-zero torque, asymptotically exact CDT shows a threshold torque for the nucleation of dislocations and it also shows the distribution of dislocation under certain torsion, which agrees well with the result by Weinberger. If the energy dissipation can‘t be neglected, it alters the distribution of dislocations, where a new dislocation-free zone is added. Size effect can be observed and the distribution of dislocation in different length scales are displayed in the end.

Automated modeling of creep in poly-crystalline Nickel-based superalloys

L. Munk (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), S. Beese (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), S. Löhnert (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 12:10

Throughout the last 60 years, nickelbased superalloys have been the standard high-temperature material used in mobile and stationary gas turbines. As dictated by thermodynamics, the main route to more fuel efficient turbines is the increase of operating temperatures. Higher temperatures necessitate further optimizations of those alloys, foremost, improving their creep-resistance. Creep denotes a macroscopic, permanent change of shape which, amongst other effects, stems from thermally and mechanically induced dislocation movement.

The key microstructural feature of most modern alloys are particles of the L12-ordered $\gamma\prime$ phase which are embedded into the nickel-based matrix. Most importantly, these particles are impenetrable to single matrix-dislocations. Dislocations within the nickel-matrix have to either climb and bypass $\gamma\prime$-particles or form ribbons of multiple dislocations which are able to cut through particles [1]. This leads to numerous dislocation effects encountered in such microstructured alloys that are still subject of ongoing research. A wealth of different material modeling-approaches exist in the literature that try to capture the creep behavior which is strongly anisotropic. Due to the multiscaled nature of the physical problem, most crystal plasticity approaches are phenomenological and, thus, rely on many parameters. Finding suitable parameters that capture experimental results becomes a challenge.

A large deformation crystal plasticity framework has been set up which allows for an efficient comparison of different, phenomenological material formulations. This has been achieved by the use of AceGEN. The software generates highly optimized Fortran-code (or C-code) of tangents in analytical form from symbolic tensorial equations. The generated tangent-subroutines are linked into a FEAP element and artificial microstructures are generated with Neper [3]. The polycrystalline aggregate is subjected to a constant load which induces plastic flow for a defined period of time. First numerical results have been obtained for artificially generated microstructures. In future work, a variety of flow rules, dislocation density based (cross-) hardening and parameters can be studied in a unified way [2].

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S 7: Coupled problems

Organizers: Ralf Jänicke (Chalmers University of Technology)
Detlef Kuhl (University of Kassel)

S 7a : Coupled problems

Tuesday 14:00 - 16:00 Marienstr. 13, Ground floor, Lecture hall A
Chair: Ralf Jänicke (Chalmers University of Technology)

Stable computational methods for strongly coupled porous media

C. Linder (Stanford University), A. Krischok, B. Dortdivanlioglu 14:00

The modeling of the interaction between the solid skeleton and an inter-penetrating fluid in porous materials has been a highly active field of research since the early defining works by Biot. In the context of the finite element method it has been recognized early that in highly coupled situations the satisfaction of the well-known *inf-sup condition* is mandatory for mixed formulations and that the same interpolation schemes that guarantee stability in cases such as Stokes flow or incompressible elasticity provide stable results in poroelasticity as well. A rigorous mathematical proof of certain elements is however unfeasible in many cases and numerical tests have been proposed to judge whether a proposed interpolation scheme is reliable [1]. While this test has been successfully evaluated for standard cases such as Stokes flow, an evaluation for poroelastic problems remains unsatisfactory [2].
This contribution presents ideas how a numerical test can be evaluated successfully in the case of poroelasticity to judge whether a novel interpolation scheme is reliable and hence guaranties uniqueness and necessary stability estimates. Based on these observations we evaluate a number of recent schemes that have recently been proposed in our research group. We present a novel low-order mixed finite element formulation based on an incompatible strain enhancement that provides inf-sup stability while preventing well-known hourglass modes in the limit of large deformations [3, 5]. In addition, in the context of isogeometric analysis we prove the stability of a variety of interpolation schemes based on degree-elevated methods and subdivision-based methods in numerical tests [5] to provide alternatives to classical schemes that, while stable in classical finite element schemes, can fail to provide inf-sup stability. The capability of the proposed schemes is underlined in exemplifying numerical examples including the consolidation of saturated soil under footings and swelling tests of polymeric gels.

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Multiphysics of Tribocontacts

G. Ostermeyer (TU Braunschweig), G. Bräuer (TU Braunschweig), J. Merlis (TU Braunschweig), P. Kaestner (TU Braunschweig), C. Kipp (TU Braunschweig) 14:20

Friction currently remains a phenomenon that is not yet completely understood. Many studies have been carried out which analyze or characterize individual aspects of specific material pairings. In practice, extrapolations of these results can only be used within very narrow application fields to predict the tribological behavior of a contact.
Brakes introduce a specialized tribological contact. As an element of both comfort and safety in the automobile world, they are capable of generating extreme dissipation rates. Recent investigations, particularly in the high-load range, show surprisingly acute variations of physical, chemical and thermal interactions on all length and time scales, which decisively influence the macroscopic properties of the contact. These processes cause the frictional properties of local microcontact surfaces to change, and even tangential vibrations on the bodies' contact surfaces can occur. As a result, the macroscopic coefficient of friction as a sum of these elementary dissipation sources is, in principle, a noise-impacted quantity. Self-organization effects can cause individual dominant frequencies of the coefficient of friction, which lead to macroscopically recognizable stick-slip effects of the bodies.
A 3D model of a unit cube of material has been developed, in which seven main components of modern brake pads and air (porosity) are integrated, broken down into elementary volumes with 50-micrometer side lengths. The size, frequency and spatial distribution of each component within the brake pad are taken into account based on common industry usage. The mechanical and thermal properties of these materials are integrated into the simulations. The aforementioned surface dynamics with locally distributed, dissipation-driven energy sources are to be implemented with this cube.

The mechanical and thermal energies are distributed among various contact structures, which come about as a result of transport and erosion processes along with chemical reactions.
This work describes the first results of a coupling of analysis and measurement of boundary layer chemistry and boundary layer physics.

Time-dependent swelling behavior of chemically stimulated hydrogels under mechanical constraints

P. Leichsenring (TU Dresden, Institut für Festkörpermechanik), T. Wallmersperger (TU Dresden, Institut für Festkörpermechanik) 14:40

Charged Hydrogels are ionic polymer gels and belong to the class of smart materials. They are multiphasic materials which consist of a solid phase, a fluid phase and an ionic phase. Therefore hydrogels exhibit a distinct viscous material behavior and, due to the presence of electric charges, they are responsive to external chemical or electrical stimuli. On the macroscopic scale, the response is governed by the reversible release or absorption of water which in turn leads to a decrease/increase of mass and a respective volume change. Many applications, in sensoric and actuatoric systems, embed hydrogels to enhance functionality or deploy them in complex environments, e.g. in the vascular system of mammals. For the further design of novel systems sensor or actuatoric systems, a numerical model of the coupled chemo-electro-mechanical model is developed.
The complex interaction of the moving constituents is captured by a statistical homogenization based on the Theory of Mixtures. By incorporating the saturation condition, a representative volume element is defined by the superposition of the fluid phase, the ionic phase and the solid phase. This definition – and a quantification based on the concept of volume fractions – is the fundamental concept of the Theory of Porous Media. The respective material property for the solid phase is defined by Hooke's law. The fluid phase is described as an incompressible fluid; the solid-fluid-interaction is modeled by Darcy's law. The behavior of the ionic phase is described by a Nernst-Planck-like equation.
The obtained field equations are solved time-dependent in the framework of the Finite Element Method. In the present investigations, a hydrogel block is chemically stimulated. Following the structure of sensor and actuator systems, the hydrogel swelling behavior is investigated for different configurations: (i) the free swelling behavior, (ii) the swelling behavior under mechanical restrictions and (iii) the swelling behavior under the application of external mechanical loads. The evaluation is performed by an investigation of the governing flux contributions. Finally, a comparison between the test case results is presented.

Continuum-based modeling of mortar mixtures modified with SuperAbsorbent Polymers: A multicomponent, multiphase model including internal mass exchange

M. Sauerwein (University of Stuttgart), H. Steeb (University of Stuttgart) 15:00

In mechanized tunneling a gap of 10 to 20 cm remains between the segment lining

and the surrounding soil. Immediately after mounting the segment rings, this gap should be filled with an adequate grouting mortar to stabilize the tunnel lining and to minimize settlements of the ground surface [4]. When the gap is filled out completely, a rapid evolution of the mortar's stiffness has to be ensured as soon as possible. For the purpose of accelerating the gelation process of the mortar, the innovative concept of using SuperAbsorbent Polymers (SAPs) as additives is examined. As the name suggests, SAPs have the ability to absorb many times more water than their own weight and therefore the amount of free water in the mixture can be controlled.
An extended mixture theory, allowing the phases to be composed of species [2], has been chosen as an appropriate framework for modeling a mortar mixture modified through SAPs. In order to capture the fundamental physio-chemical behavior of the material, we assume that the mixture consists of three coexisting but interacting phases, namely, mortar particles, mixing water and water absorbing polymers (SAPs). Macroscopically, the medium can be viewed as an immiscible mixture of different phases, whereas species are assumed to be miscible in the phases. Since internal mass exchange is permitted, the volume change of a particular phase can be caused by external forces and internal mass exchange. Against this background, the deformation has been multiplicatively decomposed [1]. Finally, it turns out that kinematics and mass exchange are coupled and a new quantity has been defined properly to capture the amount of absorbed water by the polymer network [3]. A strict exploitation of the entropy inequality is carried out to derive constitutive laws in a thermodynamic consistent framework. Herein, special attention is paid to the internal mass exchange and the effective stress principle, which contains also a contribution stemming from the SAP phase.

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[3] M. Ristinmaa, N.S. Ottosen, and B. Johannesson. Mixture theory for a thermoelasto-plastic porous solid considering fluid flow and internal mass exchange. *International Journal of Engineering Science*, 49:1185–1203, 2011.

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Surface Wetting with Droplets: A Phase Field Approach

F. Diewald (University of Kaiserslautern), C. Kuhn (University of Kaiserslautern), M. Heier (University of Kaiserslautern), M. Horsch (University of Kaiserslautern), K. Langenbach (Rice University), H. Hasse (University of Kaiserslautern), R. Müller (University of Kaiserslautern) 15:20

Wettability of structured surfaces, which can be investigated using molecular dynamics (MD) simulations with force fields [1], plays an important role in a variety of production processes. The high numerical costs for the MD simulations motivate the development of the presented phase field model which is linked to the MD simulations by its input parameters and allows for an investigation of larger scales.
An equation of state that corresponds to the MD simulations is used to define the free energy of the system. For this purpose, the local mass density (gas/liquid) is taken as the order parameter of the phase field model. The model allows to define specific contact angles without a geometric formulation but by including the surface tension between a potentially structured solid surface and the liquid as well as between the solid and the gas phase into the free energy of the system [2]. The computational domain is discretized using finite elements. Equilibrium droplet shapes and wetting conditions are computed by an Allen-Cahn evolution equation which by itself does not conserve the liquid volume. To ensure a global mass conservation (and thereby a liquid volume conservation) a global Lagrange multiplier is introduced. In order to extend the model to dynamic droplet simulations, the order parameter can be coupled to a velocity-density formulation of the Navier-Stokes equations.
The presentation covers details of the algorithmic implementation and the pertinency of the approach is demonstrated by illustrative examples.

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[2] M. Ben Said, M. Selzer, B. Nestler, D. Braun, C. Greiner, H. Garcke: A Phase-Field Approach for Wetting Phenomena of Multiphase Droplets on Solid Surfaces, *Langmuir*, 30(14), 4033-4039 (2014).

A Three stage Spray Drying Model for Zeolite 4A - Water Suspensions

M. Hribersek (University of Maribor), G. Sagadin (Silkem d.o.o.), T. Gomboc (University of Maribor), M. Ramšak (University of Maribor), M. Zadravec (University of Maribor) 15:40

The contribution deals with multi stage spray drying model of zeolite 4A suspension. The model builds on upgrading the single stage spray drying model, as used in majority of CFD codes, to a multistage drying model, suitable for the implementation in a multiphase Lagrange-Euler CFD code. In the model, the first stage describes drying of surface moisture, followed by the second stage, in which the moisture in the porous interior of the drying particle is removed. The second stage is governed by the Stefan diffusion model. The removal of the remaining adsorbed moisture in the zeolite crystals is modeled in the third stage by a kinetic model, implementing the temperature vs. moisture gradient data, obtained from the thermogravimetry data for zeolite 4A-water system. The multistage drying model is validated by comparing computational results for the particle, immersed in the drying air under varying process conditions alongside

typical particle trajectories, obtained from the CFD analysis of a pilot scale dryer. The results obtained from the numerical model are compared with experimental results, obtained from performing several tests on the pilot scale spray dryer, and confirm the applicability and physical correctness of the proposed model.

S 7a : Coupled problems

Tuesday 16:30 - 18:30 Marienstr. 13, Ground floor, Lecture hall A
Chair: Jörn Mosler (TU Dortmund)

A coupled phase transformation and solute diffusion model for bainitic transformation

M. Düsing (Universität Paderborn, Lehrstuhl für Technische Mechanik), R. Mahnken (Paderborn University) 16:30

The bainitic transformation is one of the most complex transformations in steel. The microstructure consists of bainitic ferrite, carbides and (residual) austenite. The transformation from austenite to bainitic ferrite is assumed to be displacive [1] in contrast to the perlitic growth which is highly dependent on the carbon movement and therefore is ranked as a diffusive transformation. However the movement of the carbon is of great importance for the overall bainitic transformation, considering the precipitation of carbides. The growth of the bainitic ferrite leads to a supersaturated phase, so that in lower bainite the carbon within the ferrite separates [1] and precipitates as carbides. Furthermore some carbon atoms succeed in leaving the ferrite and enrich the carbon concentration of the surrounding austenite. This may lead to carbides close to the interface between ferrite and austenite but may also stop the transformation from austenite to bainitic ferrite and produce residual austenite.
In this work the above described mechanism is characterised by a system of partial differential equations, namely a multiphase Ginzburg-Landau and an extended Cahn-Hilliard equation for the diffusion of carbon are coupled to simulate the evolution of bainite. The derivaton of this system is based on a thermodynamic framework [2] of generalized stresses as introduced by Gurtin [3]. The key aspects of the thermodynamic framework are generalized stresses and microforces which perform work in conjunction with derivatives of the phase-field variables and the carbon concentration. The framework distinguishes between basic balance laws which are universal and constitutive equations which depend on the specific material. The Clausius-Duhem inequality is used to impose restrictions to the constitutive equations. The numerical examples show the qualitativ mechanism of the bainitic transformation as discussed above.

[1] Bhadeshia, H. K. D. H. *Bainite in steels*, The Institute of Materials, Cambridge, Second Edition (2001).

[2] Düsing, M. and Mahnken, R. A thermodynamic framework for coupled multiphase

Ginzburg-Landau/Cahn-Hilliard systems for simulation of lower bainitic transformation *Arch. Appl. Mech.* (2016) 86 (12):1947–1964 (2016).

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Thermomigration in binary alloys

S. Schuß (University of Siegen), C. Hesch (University of Siegen), K. Weinberg (University of Siegen) 16:50

Solders are used to connect suitable metals and alloys such as copper, bronze, silver, aluminum but also iron, by combining their surfaces as a melt and solidifying after cooling. In flip chip modules arrays of solder bumps are used to interconnect semiconductor devices, such as IC chips and microelectromechanical systems to external circuity. With the trend toward higher integration and further miniaturization in the microelectronic industry the cross sectional area of the conductive lines within electronic packages has decreased drastically. Due to different electrical resistances of the conducting paths on the chip and on the circuit board the temperature on the chip side can be significantly larger than the temperature on the board side. This inevitably leads to a considerable temperature gradient across the solder bumps providing a driving force to cause thermomigration. Thermomigration can produce significant redistribution of elements and constituent phases in single and two-phase alloys. Microstructural changes such as phase decomposition and coarsening may, of course, affect the overall properties of the alloy which degrade the stability and performance of components.

In our contribution we present a model describing the evolution of the composition profile and microstructure in two phase alloys in the present of a temperature gradient caused by the Joule-heating effect. The model takes into account both, the Soret effect and his counterpart the Dufour effect which is an energy flux due to a mass concentration gradient. There are three important parameter used in the model: the Gibbs' free energy density, the mobility of atoms presented and their heat of transport. Here we will focus on a Sn-Pb alloy and outline the modelling of these parameters as sufficiently smooth functions in mole fraction and temperature.

The model consists of two nonlinear fourth order partial differential equations. Consequently, the variational formulation of the problem mandates approximation functions which are at least C^1-continuous. In order to fulfill this requirement a B-Spline based finite element scheme is provided. One of the main advantages of B-Splines is the possibility to represent complex geometries exactly. However, since B-Spline bases are non-interpolatory boundary conditions can not be treated in a straight forward manner. For this reason we finally discuss the implementation of boundary conditions in the presented framework. Concluding computational studies of thermomigration events within Sn-Pb alloys will corroborate the quality of our model.

[1] Schuß, S., Hesch, C. and Weinberg, K. *Thermomigration in SnPb solders: Material model.* In preparation.

[2] Schuß, S., Hesch, C. and Weinberg, K. *Thermomigration in SnPb solders: Numerical aspects*. In preparation.

Diffusion induced void nucleation

M. Werner (Uni Siegen), K. Weinberg (Universität Siegen) 17:10

Towards a simple model for void-based fatigue prediction, we investigate the interaction of voids by using a multi-field ansatz. We couple the concentration field c with an indicator field η, where the latter is assigned with damage. The interaction potential manifests the two stable phases at $(c_1, \eta_1) = (0, 0)$ and $(c_2, \eta_2) = (1, 1)$ by construction. A similar ansatz has been already made to account for long range interactions. To make it thermodynamically consistent, in a further step the configurational entropy is implemented in a logarithmic form, which requires a degenerate model for the mobility. In general, the particles size affects the eutectic temperature point and thus the Gibbs energy. Nevertheless, it has been shown that the interfacial energy coefficient is independent of voids size, but rather depends numerically on the mesh size, which is used in the model presented here. Both governing equations follows a Cahn-Hilliard-type and a Allen-Cahn-type equation, respectively and are solved using a NURBS-based ansatz.

A generic variational constitutive update based on hyper-dual numbers: Application to thermomechanical gradient enhanced plasticity

V. Fohrmeister (Institute of Mechanics, TU Dortmund), A. Bartels (Institute of Mechanics, TU Dortmund), J. Mosler (Institute of Mechanics, TU Dortmund) 17:30

Within this work, a generic variational framework for thermomechanically coupled plasticity theory is presented, cf. [1]. This framework is based on so-called variational constitutive updates. To be more precise, an incremental potential and a sufficient parametrization of the internal variables is proposed such that the stationary points of the aforementioned potential automatically fulfill the underlying balance laws and the constitutive equations. In order to solve the resulting equations numerically, exact numerical differentiation by means of hyper-dual numbers is employed, see [2]. That is, the solution is computed in an automated manner, which results in fast development times. As a prototype model, thermomechanically coupled gradient enhanced plasticity theory is considered and implemented in line with [3]. The capabilities of the constitutive model as well as the robustness and accuracy of the algorithmic formulation are shown by means of several numerical examples including thermal necking.

[1] A. Bartels, T. Bartel, M. Canadija and J. Mosler. In: JMPS., 82: 218-234, 2015.

[2] J. A. Fike and J. J. Alonso. In: Paper 886, 49th AIAA Aerospace Sciences Meeting, 2011.

[3] B. Dimitrijevic and K. Hackl. In: Int. J. Numer. Methods Biomed. Eng., 27:1199-1210, 2011.

Diffusion and trapping of lithium ions in SiOC nanocomposites

P. Stein (TU Darmstadt), B. Xu (Technische Universität Darmstadt) 17:50

Nanocomposites of SiOC are an attractive anode material for Li-ion batteries in high-temperature applications. They exhibit a capacity three times larger than current commercial graphite anodes. Other than Si (with an even higher theoretical capacity), this material system does not show large deformations during a charge-discharge cycle, and no mechanical degradation has been observed experimentally.
These composites consist of an amorphous network of Si-O-C, interpenetrated by free carbon. The amount of free carbon thereby determines the capacity of the composite. It does, however, also affect the cycle stability of the material. Compounds with low carbon content or with carbon fractions above a certain threshold suffer from significant irreversible lithium storage. This effect is assumed to be related to the electrical conductivity of the composite.
In this talk we describe a coupled electro-chemical model for diffusion and trapping of Li ions in SiOC nanocomposites. Mobile and immobile ions as well as electrons are thereby regarded as individual species. Using this model, we demonstrate the influence of carbon content on the immobilization behavior.

Modeling of the deformation-dependent fluid flow in the fibrous gas diffusion layer of fuel cells

M. Chaaban (RWTH Aachen, Institute of General Mechanics (IAM)), Y. Heider (RWTH Aachen, Institute of General Mechanics (IAM)), B. Markert (RWTH Aachen, Institute of General Mechanics (IAM)) 18:10

Electrochemical energy devices, such as fuel cells, electrolysers and batteries, belong to a promising alternate, non-polluting energy conversion technology, which can be employed in broad areas such as in portable, stationary, and transportation applications. These devices are mainly constructed of a porous layers assembly subjected to mechanical loadings, which operate in a mechano-electro-chemical process, in order to generate electricity. During manufacturing of the fuel cell, the gas diffusion layer (GDL), the main gateway of the "fuel" from the gas channels to the catalyst layer, witnesses compression of its fibrous microstructure and a change of its porous media and transport properties. As a result, the supply of gas would be altered and, as a consequence, the fuel cell's performance on the system's level [1].
To this end, this preliminary study will numerically model the transport in the porous layer based on the fundamentals of multiphase continuum mechanics in relation to the Thoery of Porous Media (TPM) [2]. The model will be able to mimic the transport in porous media and the change of the microstructure porous media properties under compression. The TPM proceeds from the homogenization of the fibrous microstructure and the smearing out of the real microstructure through the considered domain on the basis of an averaging process. In other words, the idealization of multiphasic materials is based on superimposed continua with internal interactions as the result of the averaging process. The compression of the GDL leads on the microscopic level to deformation and re-orientation of the fibers and reduction of the transport capability through the micro

channels, which can be studied and quantified using micro-CT images. The numerical findings will be validated with respect to the experimental extractions of the material characteristics.

[1] Tötzke, C., Gaiselmann, G., Osenberg, M., Bohner, J., Arlt, T., Markötter, H., Hilger, A., Wieder, F., Kupsch, A., Müller, B.R., Hentschel, M.P., Bahnart, J., Schmidt, V., Lehnert, W., Manke I.: *Three-dimensional study of compressed gas diffusion layers using synchrotron X-ray imaging*, Journal of Power Sources 253 (2014), 123-131.

[2] Markert, B.: *A constitutive approach to 3-d nonlinear fluid flow through finite deformable porous continua*, Transport in Porous Media 70 (2007), 427-450.

S 7a : Coupled problems

Wednesday 14:00 - 16:00 Marienstr. 13, Ground floor, Lecture hall A
Chair: Tobias Gleim (Universität Kassel)

A damage phase field model for pressure diffusion in fractured porous media - Computational homogenization and order reduction

R. Jänicke (Chalmers University of Technology), F. Larsson (Chalmers University of Technology), K. Runesson (Chalmers University of Technology) 14:00

At low seismic frequencies ($f < 100\,\mathrm{Hz}$) fluid-saturated fractured rocks are well-known to exhibit high attenuation of elastic waves due to pressure diffusion accompanied by a local redistribution of pore fluid in the porous rock as well as in the fracture networks. Due to the extreme aspect ratio (quotient of fracture length over fracture opening) $a >$ 1e-5 being observed for such fractures the proper mechanical description as well as the numerical treatment of diffusion in fracture networks is delicate. In literature various approaches are available. One may distinguish between sharp interface models (hybrid-dimensional approach using surface elements, XFEM) and diffuse interface models (phase-field). Whereas the sharp interface models allow for numerically efficient computations they suffer, first, from the highly demanding discretization of 3D fracture network topologies and, second, from the difficulty to describe fracture propagation. The phase-field models on the contrary require a rather fine yet simple discretization of the fracture zone. However, they provide a very natural way to model the evolution of fracture networks in fluid-saturated rocks.

In this contribution, we review poroelastic fracture phase-field models available in literature [1,2] and present a novel double-porosity fracture phase-field model in the context of the Theory of Porous Media. We qualitatively and quantitatively investigate the coupling mechanisms and diffusion processes predicted by all these models in a set of numerical benchmark experiments for non-evolving fracture networks. Finally, we

introduce a computational homogenization and order reduction technique to derive the viscoelastic properties of a macroscopic substitute model [3]. This procedure enables us to monitor seismic attenuation due to pressure diffusion in fracture networks during hydraulic fracturing.

[1] Mikelić A., M. Wheeler & T. Wick [2015]. 'Phase-field modeling of a fluid-driven fracture in a poroelastic medium' *Computat. Geosci.*, 19, pp. 1171–1195.

[2] Miehe C. & S. Mauthe [2016]. 'Phase Field Modeling of Fracture in Multi-Physics Problems. Part III. Crack Driving Forces in Hydro-Poro-Elasticity and Hydraulic Fracturing of Fluid-Saturated Porous Media' *Comput. Meth. Appl. Mech. Eng.*, 304, pp. 619–655.

[3] Jänicke R., F. Larsson, K. Runesson & H. Steeb [2016]. 'Numerical identification of a viscoelastic substitute model for heterogeneous poroelastic media by a reduced order homogenization approach' *Comput. Meth. Appl. Mech. Eng.*, 298, pp. 108–120.

A phase-field model of hydraulic fracture in saturated binary porous media

M. Pise (Universität Duisburg-Essen), J. Bluhm (Universität Duisburg-Essen), J. Schröder (Universität Duisburg-Essen) 14:20

In many fields of engineering, especially in geo sciences and rock mechanics, the theoretical and numerical modeling of hydraulic fracturing of porous materials plays an important role. Hydraulic fracturing is a well stimulation technology in which porous materials are fractured by a pressurized liquid. The process involves the pressure injection of the fracking fluid (primarily water, often enriched with filling materials and thickening agents) and accompanied by crack nucleation and propagation as well as mass transport. In this contribution, a macroscopic model based on the Theory of Porous Media (TPM) is presented in view of the description of the aforementioned phenomena. The aim is to increase the permeability of the reservoir rock formations, whereby the situated gas or oil in the rock can be flow more easily and stable to a borehole and the flow rate increase, see [1]. For simplification an incompressible binary model consisting of the phases solid and liquid is used. Attention is paid to the description of the damage of the elastic solid phase. The development of the damage parameter is controlled by an evolution equations, which corresponds to known diffusive phase field models within a continuum mechanical framework. A phase-field model for rate-independent crack propagation is given in [2]. Therein, they presented a new approach to the construction of phase-field models of fracture by using an additive decomposition of the elastic energy so that a energy-release-driven fracture occur due to tension only. Based on the Theory of Porous Media, extended by the phase-field theory, [3] and [4] presented an incompressible binary model (elastic solid and viscous fluid) for the numerical simulation of hydraulic fracturing. A numerical example from [5] is solved which shows that the simplified model is indeed capable of simulating hydraulic fracturing processes inside a rock specimen.

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[3] B. Markert and Y. Heider. Coupled multi-field continuum methods for porous media fracture. In M. Mehl, M. Bischoff, and M. Schäfer, editors, *Recent Trends in Computational Engineering - CE2014*, volume 105 of *Lecture Notes in Computational Science and Engineering*. Springer, 2015.

[4] W. Ehlers and C. Luo, A phase-field approach embedded in the theory of porous media for the description of dynamic hydraulic fracturing. *Computer Methods in Applied Mechanics and Engineering*, 315:348-368, 2017.

[5] L. C. Li, C. A. Tang, G. Li, S. Y. Wang, Z. Z. Liang, and Y. B. Zhang. Numerical simulation of 3d hydraulic fracturing based on an improved flow-stress-damage model and a parallel fem technique. *Rock Mechanics and Rock Engineering*, 45:801-818, 2012.

Efficient numerical modelling of hydro-mechanics in fractures using a hybrid-dimensional approach and non-conformal mesh coupling

P. Schmidt (Uni Stuttgart - MIB), H. Steeb (Uni Stuttgart - MIB) 14:40

The investigation of subsurface fluid flow is of interest in particular to determine characteristics of matter and heat transport below the earth surface and the characteristics of the underground storage of fluids. Classical approaches such as extended diffusion equations are lacking to capture key phenomena such as inverse water-level fluctuations (Noordbergum effect) obtained during pumping tests performed on aquifers [Rodrigues, 1983, Horne, 1995]. Another well-known approach in order to model the aforementioned phenomena is the Biot's theory [Biot, 1941]. Nevertheless explicit discretization of the fracture geometry is computationally expensive and fails for fractures with a high aspect ratio [Vinci, 2014]. Hence a recent study by C. Vinci [Vinci et al., 2015] discusses the importance of hydro-mechanical coupling of fluid-pressure variations and the deformation of the surrounding rock using a lower dimensional description of the fracture flow which is consistently coupled to the porous bulk material. So far the coupling of both descriptions has not been implemented efficiently and ends up in limitations due to discretization issues. This problem is resolved in this work by using an efficient numerical implementation in the Dune framework [Blatt et al., 2016] and non-conformal mesh computations. A theoretical background of the implemented model is given and the implementation strategy is introduced along with results of benchmark boundary value problems.

Numerical investigation of the effective Skempton coefficient in fluid-saturated fractured rock

N. Pollmann (Institute for Computational Engineering, Ruhr-Universität Bochum), R. Jänicke (Department of Applied Mechanics, Chalmers University of Technology), J. Renner (Institute of Geology, Mineralogy and Geophysics, Ruhr-Universität Bochum), H. Steeb (Institute of Mechanics (CE), University of Stuttgart) 15:00

Characterization of hydro-mechanical processes in reservoir rock is an essential issue for many seismic engineering applications such as characterization of subsurface fluid flow or geothermal exploitation. A special case of wave propagation is the investigation of fractured porous rock. For geothermal problems, the role of fractures as storage and transport components of a fracture network are highly important. We, therefore aim to model the storage and transport processes in fracture networks numerically. Thus, we create synthetic periodic fracture topologies in porous fluid-filled rock to mimic geological in-situ situations. These fractures exhibit high-aspect-ratio geometries, i.e. they constitute thin and long hydraulic conduits.

In the present contribution we focus on the investigation of the effective Skempton coefficient $\bar{B}$ for such complex fracture networks in porous rock. The effective Skempton coefficient is defined as the ratio of induced pore pressure and the confining pressure for undrained boundary conditions. Using a computational homogenization approach we evaluate the confining pressure as the negative volume average of the total mean stress. Similarly, we compute the effective pore pressure in terms of the volume averaged fluid pressure in the fractured rock. Thus, the effective Skempton coefficient allows for the interpretation of hydraulic properties of fluid-saturated fractured rock on the geological scale. We compare the numerical procedure to experimental setup and highlight the deficiencies of the latter. Altogether, the proposed concept of the efficient Skempton coefficient based on numerically evaluated volume averages helps to generate a better understanding of the interactions of local transport processes and the geological model. It, therefore, represents a significant enhancement of the currently available techniques.

A coupled SPH-Phase Field approach applied to hydraulic fracturing

M. Osorno (Universität Stuttgart), H. Steeb (Universität Stuttgart) 15:20

Simulation of fracture initiation and propagation using classical mesh-based methods involves computationally expensive operations for geometry pre-processing and remeshing. To overcome this difficulties we propose to use the mesh-less Smoothed Particle Hydrodynamics (SPH) method to model fracturing processes in biphasic poroelastic media. SPH is a Lagrangian method highly suitable for large deformations [1]. In the present approach we assume rigid solid grains and negligible inertia effects of the pore fluid [2]. We present simulations of various consolidation problems and validate the pressure diffusion results against the analytical solution.

Furthermore we extend the proposed approach to model fracture initiation and propagation, by coupling the SPH model with the Phase Field method [3]. The proposed hybrid method overcomes the instability problems that can present SPH due to kernel

incompleteness during fracture initiation. The proposed coupled method is first tested with single phase media. Second, we present the comparison between the SPH and the coupled SPH-Phase field models.
We investigate problems in a geothermal exploration framework, which requires the simulation of considerably large domains, therefore we implement the computational model in a massive parallel scheme.

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[3] M. Hofacker and C. Miehe (2012). Continuum phase field modeling of dynamic fracture: variational principles and staggered FE implementation. *International Journal of Fracture*, 178(1-2), 113-129. doi:10.1007/s10704-012-9753-8

On the numerical modeling of initiation of sediment transport using Smoothed Particle Hydrodynamics

N. Falkner (Universität Stuttgart), H. Steeb (Universität Stuttgart) 15:40

Mobilization of solid particles at the interface between a porous and a free flow domain is a relevant subject in many fields of mechanical, civil and environmental engineering. One example is the initiation of sediment transport as it appears in river beds. To approximate this initiation state, various theoretical models exist. Most of these models approximate critical values for the interfacial velocity or the interfacial shear stresses at the interface between a porous and free flow domain. Common approaches use two-domain formulations as in [1] or one-domain formulations as in [2]. The named approaches [1, 2] were compared with Direct Numerical Simulations in [3]. The results of these simulations showed that the theoretical models often underestimate the occurring velocities at the interface and therefore critical velocities to initialize the motion of single grains can be lower than predicted by theoretical approaches. Thus our aim was to extend the numerical model to 3D applications to study the fluidization of a solid grain bed with more realistic problem parameters [4].
We therefore present Direct Numerical Simulations of a Newtonian single-phase fluid with embedded solid particles to consider the flow behavior and fluid-solid interactions as occurring in sediment transport. Following the model proposed by [5] we present an implementation using the molecular dynamics particle code HOOMD-blue [6] extended for the usage of Smoothed Particle Hydrodynamics (SPH) [7, 8]. Since both the fluid and the solid domain can be discretized by particles, SPH, as a particle method of Lagrangian character, presents a good choice to model this particular non-linear problem. As a first

boundary value problem, we study the flow behavior of single and multiple spherical solid grains in a Newtonian single-phase fluid applying different boundary conditions such as gravity or shear flow. Contrary to what was shown in [5], we focus on the pore scale effects, for example the mobilization forces acting on a bed of solid grains as well as the transformation of flow behavior depending on the number of suspended particles.

[1] G. S. Beavers and D. D. Joseph. Boundary conditions at a naturally permeable wall. *J Fluid Mech*, 30:197–207, 1967. doi:10.1017/S0022112067001375.

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S 7a : Coupled problems

Wednesday 16:30 - 18:30 Marienstr. 13, Ground floor, Lecture hall A
Chair: Andreas Ricoeur (Universität Kassel)

High-Order Numerical Methods for Electromagnetic Induction

T. Gleim (University of Kassel), D. Kuhl (University of Kassel) 16:30

An important concept in metal forming processes is local heat treatment and cooling that influence local material properties, such as ductility, hardness, yield strength, or impact resistance, cf. [1]. Cold forming methods by means of electromagnetic forces are also of great scientific interest, in order to obtain special shapes and product properties, cf. [2]. To make these techniques more effective in industry, or to optimize its application, corresponding numerical simulation tools are needed.
One of the main topics of these manufacturing processes is characterized by the electromagnetic influence. These processes, in which electromagnetic induction comes into play, involve highly dynamic effects, which cannot be neglected. Thus, adequate material models as well as proper numerical schemes have to be established. Therein, the focus will be on the application of high-order accurate numerical schemes in combination with appropriate error estimators, cf. [3].
In order to be able to solve these complex industrial processes in space and time in a highly accurate manner, the corresponding physical effects need to be validated in a simulation process. Since electromagnetic effects have strong interactions and the difficulty of the problems increases rapidly with any additional complexity in the geometry, analyses for special examples with a corresponding analytical solution are required. The influences of the spatial as well as the temporal discretization with respect to the physical fields are of decisive importance.
For the spatial discretization, higher-polynomial Lagrange approaches are used, which are compared with corresponding h-studies and the analytical solution in order to assess their quality and the computational effort. In a further step, high-order accurate Galerkin time integration schemes as well as diagonally implicit Runge-Kutta methods are applied to the semi-discrete balance equation of electromagnetic induction, cf. [4, 5]. Moreover, time discretization error analyses with respect to the time integration methods are performed. The classical h-error estimator, as well as special classes of error estimators of the Galerkin time integration methods and the Runge-Kutta methods are investigated, cf. [3, 4].

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Finite element simulation of nonlinear magnetoelectric coupling and damage behaviour in multiferroic composites

A. Avakian (University of Kassel), A. Ricoeur (University of Kassel) 16:50

The coupling of magnetic and electric fields due to the constitutive behavior of a material is commonly denoted as magnetoelectric effect. The latter is only observed in a few crystal classes exhibiting a very weak coupling, mostly at low temperatures, which can hardly be exploited for technical applications. Much larger coupling coefficients are obtained at room temperature in composite materials with ferroelectric and ferromagnetic constituents. The magnetoelectric effect is then induced by the strain of matrix and inclusions converting electrical and magnetic energies based on the piezoelectric and magnetostrictive effects.
In this paper, the constitutive modelling of nonlinear multifield behavior as well as the finite element implementation are presented [1, 2]. Nonlinear material models describing the magneto-ferroelectric or electro-ferromagnetic behaviors are presented. Both physically and phenomenologically motivated constitutive models have been developed for the numerical calculation of principally different nonlinear magnetostrictive behaviors. Further, the nonlinear ferroelectric behavior is based on a physically motivated constitutive model. On this basis, the polarization in the ferroelectric and magnetization in the ferromagnetic and magnetostrictive phases, respectively, are simulated and the resulting effects analyzed. Additionally, the ferroelectric model accounts for damage due to microcrack growth. Numerical simulations focus on the calculation of magnetoelectric coupling and on the prediction of local domain orientations as well as damage processes going along with the poling process, thus supplying information on favorable electric-magnetic loading sequences.

[1] A. Avakian, R. Gellmann and A. Ricoeur, Acta Mechanica. 226, 2789-2806 (2015).

[2] A. Avakian and A. Ricoeur, J. of Intel. Mat. Sys. and Struct. 27, 2536-2554 (2016).

Numerical methods for the modeling of the magnetization vector in multiferroic heterostructures

W. Dornisch (University of Kaiserslautern), D. Schrade, R. Müller (TU Kaiserslautern) 17:10

Multiferroic heterostructures are commonly used to obtain electro-magnetic coupling effects. Thereby, the ferroelectric layer is used to control the magnetization in the ferromagnetic layer. The coupling between the layers is obtained by the mechanical coupling between the layers, which have well-defined interfaces. Within this contribution we use phase field models to define the polarization and magnetization in the ferroelectric and ferromagnetic layers, respectively. A coupling between polarization/magnetization and strains in each layer in combination with coherent deformations at the interface yields an electromagnetic coupling within the entire heterostructure. Numerical formulations for the interpolation of the polarization vector are well-defined in the literature. However,

the establishment of a consistent numerical formulation for the ferromagnetic layer, where the length of the magnetization vector has to be constant, remains a difficult task. We propose a new numerical approach for the consistent treatment of the ferromagnetic layer and provide numerical simulations which illustrate the electromagnetic coupling effect.

A Large Deformation Phase Field Approach for Magneto-Sensitive Elastomers

A. Sridhar *(Institute of Applied Mechanics (CE)), M. Keip (University of Stuttgart)* 17:30

The advancements in technology has dictated the demand for sensors and actuators that are more adaptable and effecient whilst being more reliable. Smart or functional materials have received significant attention in recent times due to this. Magneto-Rheological Elastomers (MREs) are a special class of these materials, where micron-sized ferromagnetic particles are embedded in an elastomeric matrix material. The large deformation capable by these materials coupled with their high operating frequency, makes these materials very attractive for engineering applications.

The behavior of these materials is however a complex phenomenon that spans over multiple scales. The ferromagnetic inclusions show complex magnetic domain wall motions on the micro-scale, which drives the magneto-mechanical deformations seen on the macroscopic level. To capture this behavior we propose *large deformation variationally consistent micro-magnetic framework*. The *magnetization* phase field describes the evolution of the magnetic domain wall motions. The *large-deformation* theory captures the particle to particle interaction through the *magnetic self-field* that drives the mechanical deformation in the elastomer. The *rate-type saddle point variational principle* gives the celebrated *Landau-Lifshitz-Gilbert* equation for the temporal evolution of the magnetization. The proposed variational principle is a straight forward description of a magneto-mechanical coupled phase-field problem at large strains. Apropriate numerical examples are presented that showcase the capability of the framework to determine the domain wall motion in ferromagnetic materials, and in turn determine the effect of particle shape and volume fraction in the macroscopic behavior of MREs.

1. M.-A. Keip & M. Rambausek [2016], "A multiscale approach to the computational characterization of magnetorheological elastomers", Int. J. Numer. Meth. Engng 107, 338–360,

2. A. Sridhar, M.-A. Keip, C. Miehe, *Homogenization in Micro-Magneto-Mechanics*, Computational Mechanics, 58, 151–169, 2016.

3. C. Miehe, D. Vallicotti, S. Teichtmeister, *Homogenization and multiscale stability analysis in finite magneto-electro-elasticity. Application to soft matter EE, ME and MEE composites*, Computer Methods in Applied Mechanics and Engineering, 300, 294–346, 2016.

On variationally-consistent homogenization approaches in multi-phase magnetic solids

B. Kiefer (TU Bergakademie Freiberg), T. Bartel (TU Dortmund) 17:50

The prediction of effective material behavior based on the knowledge of phase-specific geometrical, distributional and constitutive properties available on a lower scale by means of adequate homogenization concepts is a classical problem in solid mechanics. For the purely mechanical case it has also been established in the literature that the conventional averaging methods employed in micromechanics—e.g. Taylor/Voigt, Reuss/Sachs assumptions—are not only interpretable as energetic bounds in the linear elastic case, but, in fact, are consistent with general variational principles of *energy relaxtion*. Considering incremental settings, such principles are applicable to the modeling of physically and geometrically nonlinear as well as inelastic material behavior.
In this contribution we discuss novel ideas on how to define analogous notions of energy-relaxation-based homogenization for the constitutive modeling of multi-phase magnetic materials. In particular, Taylor/Voigt, convexification and (partial) sub-rank relaxation concepts will be discussed with respect to the magnetic phase boundary compatibility and balance assumptions they imply, and their relation to the conditions set by Maxwell's laws of magnetostatics. While currently restricting our attention to multi-phase solids in which each of the phases can still be regarded as a *macroscopic* magnetic material [1], an outlook is given on the implications of this novel approach on micromagnetics-based modeling. Moreover, on-going research on the generalization of the suggested principles to magneto-mechanical coupling is discussed.

[1] C. Miehe, B. Kiefer, D. Rosato, An incremental variational formulation of dissipative magnetostriction at the macroscopic continuum level, *International Journal of Solids and Structures*, 48(13):1846–1866, 2011.

Magneto-electro-active polymers: material properties and structural effects

M. Rambausek (University of Stuttgart), M. Keip (University of Stuttgart) 18:10

Materials with magneto-electric (ME) coupling allow for, e.g., ME random access memories and electrical magnetic-field sensors. Since single-phase materials exhibit extremely weak coupling, ME composites become relevant. As an alternative to classical approaches [6, 3], we discuss a new realization of ME coupling based on *soft-matter* composites [5]. Those have some advantages compared with classical composites: They are less fragile, their manufacturing is straight-forward, and their constituent phases are cheap.
In this contribution, we first employ computational homogenization to analyze the effective properties of ME composites [4]. Then we go one step further and present multiscale simulations of macroscopic ME sensor devices. In such a situation, the overall response of a ME structure is determined by two factors: besides the effective material properties of the composite, the magneto-electro-mechanical interactions of the macroscopic structure with its surrounding play an equally important role, as demonstrated

in [2, 1] for magnetorheological elastomers. Motivated by these complications, having both microscopic and macroscopic results at hand, we finally relate the overall response of the macroscopic ME sensor to its effective material properties *and* int macroscopic shape. By that, we try to shed some light on the influence of material properties on the one hand, and macroscopic structural effects on the other hand.

[1] M.-A., Keip and M. Rambausek *International Journal of Solids and Structures, submitted*, 2016.

[2] M.-A. Keip, and M. Rambausek. *International Journal for Numerical Methods in Engineering*, 107(4):338–360, 2016.

[3] J. Schröder, M. Labusch and M.-A. Keip. *Computer Methods in Applied Mechanics and Engineering*, 302:253–280, 2016.

[4] C. Miehe, D. Vallicotti, and S. Teichtmeister. *Computer Methods in Applied Mechanics and Engineering*, 300:294–346, 2016.

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S 7a : Coupled problems

Thursday 14:00 - 16:00 Marienstr. 13, Ground floor, Lecture hall A
Chair: Marc-André Keip (Universität Stuttgart)

Computational Multi-Scale Stability Analysis of Periodic Electroactive Polymer Composites at Finite Strains

E. Polukhov (University of Stuttgart), D. Vallicotti (University of Stuttgart), M. Keip (University of Stuttgart) 14:00

Dielectric materials such as electro-active polymers (EAPs) belong to the class of functional materials which are used in advanced industrial environments as sensors or actuators and in other innovative fields of research. Driven by Coulomb-type electrostatic forces EAPs are theoretically able to show deformations of several hundred percents. These devices become practical as soon as the material is robust, reliable and long living. However, large actuation fields and different types of instabilities prohibit the ascend of these materials. One distinguishes between *global structural instabilities* such as buckling and wrinkling of EAP devices, and *local material instabilities* such as limit- and bifurcation-points in the constitutive response. Numerically predicting global and local instabilities is a necessary, however demanding task for designing optimal devices. To incorporate microscopic phenomena of electro-mechanically coupled composite materials into the overall macroscopic response we employ *computational homogenization*

onto periodic microstructures. This approach requires the use of representative volume elements (RVEs) which imposes additional difficulties for microscopic stability analyses. It was shown, that bifurcation type instabilities of the microscale may alter the critical number of unit cells in an RVE. Based on the work of [1] and [2] among others, we propose criteria for macro- and microscopic instabilities based on the loss of ellipticity for composite materials with soft and stiff electro-active inclusions and employ a *Bloch-Floquet wave analysis* to determine long and short wavelength microscopic instabilities, ultimately leading to the computation of new critical periodicities of the RVE. Starting point is a *pure minimization principle* of electro-elasto-statics based on an electric vector potential and the scale-bridging is achieved by a Hill-Mandel macro-homogeneity condition yielding appropriate boundary conditions for the surface of the microstructure, as proposed in [3]. A macroscopic driver procedure is employed to impose loading conditions onto the microscale. In an accompanying procedure the Bloch-Floquet wave analysis shows the instability surfaces for certain loading paths and reveals the new critical periodicities.
Numerical examples validate the theory and show the critical periodicities of the RVE. By a consecutive Finite Element analysis bifurcation paths are followed and deformation modes are displayed.

1. G. Geymonat, S. Müller, N. Triantafyllidis, *Homogenization of nonlinearly elastic materials, microscopic bifurcation and macroscopic loss of rank-one convexity*, Archive for Rational Mechanics and Analysis, 122, 231-290, 1993.

2. K. Bertoldi, M.C. Boyce, *Wave propagation and instabilities in monolithic and periodically strctured elastomeric materials undergoing large deformations*, The American Phsysical Society, 78, 184107, 2008.

3. C. Miehe, D. Vallicotti, S. Teichtmeister, *Homogenization and multiscale stability analysis in finite magneto-electro-elasticity. Application to soft matter EE, ME, and MME composites*, Computer Methods in Applied Mechanics and Engineering, 300, 294–346, 2016.

A polarisation based approach to model strain dependent electrostatic pressure of dielectric elastomer actuators

T. Schlögl (University of Erlangen-Nuremberg), S. Leyendecker (University of Erlangen-Nuremberg) 14:20

Dielectric elastomer actuators (DEAs) are composed of an elastic dielectric material that is sandwiched between two compliant electrodes. When the electrodes are charged by applying a voltage, charges with opposite signs attract each other, leading to a contractive force also known as electrostatic pressure. A wide-spread lumped parameter model describing the electrostatic pressure is presented by Pelrine et. al. in 1998 [1]. In Pelrine's model, the electrostatic pressure is affected by the relative permittivity of

the material, also known as dielectric constant. However, many researchers found that the dielectric constant of DEAs is not constant at all, but decreasing with increasing pre-stretch of the material (e.g. [2]). From a physical point of view, polarisation within the dielectric material is responsible for the material's permittivity and in general, polarisation is deformation dependent. In this work, an alternative modelling approach is presented, explaining the stretch dependent actuation pressure. It is shown that Pelrine implicitly assumes that the polarisation of the material is linear in the actuating electric field strength. If this assumption is modified to allow for a more general polarisation field that is based on invariants of the electromechanically coupled problem [3], a new polarisation based lumped parameter model is obtained. It is shown that this new model fits experimental data found in literature quite well.

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[3] A. Dorfmann, R.W. Ogden. Nonlinear electroelasticity. Acta Mechanica, 174:167-183, 2005.

A condensed approach to model the constitutive behavior of multiphase ferroelectric and multiferroic materials

S. Lange (University of Kassel), A. Ricoeur (University of Kassel) 14:40

Ferroelectric as well as ferromagnetic materials are widely used in smart structures and devices as actuators, sensors etc. To model their nonlinear behavior, a variety of models has been published in the past decades, e.g. [1]. Most of the models that have been developed were implemented within the framework of the Finite Element Method (FEM), e.g. [2, 3]. The implementation of a discretization scheme is going along with a high computational effort and the solution of the boundary value problem (BVP) requires high computational costs. Most investigations, however, are restricted to simple BVP under uniaxial or biaxial loading and their goal is the calculation of hysteresis loops or to determine e. g. electromechanical coupling effects. In [4] the so-called condensed method (CM) is introduced to investigate the polycrystalline material behavior at a macroscopic material point without any kind of discretization scheme. The CM is able to calculate hysteresis loops as well as residual stresses as a result of domain wall motion. Based on the condensed theory, a high cycle fatigue model is introduced in [5] to predict the life time under combined electromechanical loading. Besides classical ferroelectrics, other fields of application of the CM have been exploited, e.g. ferromagnets, ferroelectric-ferromagnetic composites or ferroelectrics with phase transition. In this paper the focus is on multiphase materials. Here, two different methods are presented:

First, the CM is extended to nonlinear ferromagnetic material behavior to investigate the magnetoelectric coupling in a multiferroic composite, where a microscopic material point is either ferroelectric or ferromagnetic. Secondly, rhombohedral unit cells are implemented within the framework of the CM. A multiphase problem is then considered at each microscopic material point, to examine the phase transition at the morphotropic phase boundary (MPB).

[1] Hwang, S. C., Lynch, C. S. and McMeeking, R. M., Ferroelectric / ferroelastic interactions and a polarization switching model, Acta Metallurgica et Materialia 43, 1995, pp. 2073 – 2084.

[2] Avakian, A. and Ricoeur, A., Constitutive modeling of nonlinear reversible and irreversible ferromagnetic behaviors and application to multiferroic composites, Journal of Intelligent Material Systems and Structures, 2016, DOI: 10.117/1045389X16634212.

[3] Avakian, A., Gellmann, R. and Ricoeur, A., Nonlinear modeling and finite element simulation of magnetoelectric coupling and residual stress in multiferroic composites, Acta Mechanica 226, 2015, pp. 2789 – 2806.

[4] Lange, S. and Ricoeur, A., A condensed microelectromechanical approach for modeling tetragonal ferroelectrics, International Journal of Solids and Structures 54, 2015, pp. 100 – 110.

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Phase-field simulation of flexoelectricity in ferroelectrics by mixed finite element method

S. Wang (TU Darmstadt), B. Xu (TU Darmstadt) 15:00

Flexoelectricity describes the linear coupling between the electric polarization and the mechanical strain gradient or that between the mechanical strain and the polarization gradient. [1] Unlike other electromechanical coupling effects such as piezoelectricity and electrostriction, which require the non-centrosymmetric of the structure, flexoelectric effect appears in materials of any symmetry. Due to the low value of flexoelectric coefficients, the research on flexoelectricity in solids had long been overlooked, until a series of experimental observations about large flexoelectric effect of ferroelectric materials were reported by Ma and Cross in last decades. [2] The researchers are intrigued by these discoveries to study flexoelectricity and its applications, especially in nanoscale systems, which indicate bright prospect in utilizing flexoelectric effect of materials.

In this presentation, a continuum phase-field model of flexoelectricity is established in order to investigate the influence of flexoelectricity on the polarization and mechanical

properties of ferroelectric materials. To deal with the high-order nature (strain gradient) originated from the flexoelectricity, a mixed finite element treatment is utilized. [3] For the ferroelectric properties, the polarization is regarded as the order parameter in phase field simulation. The evolution of the polarization is governed by the time-dependent Ginzburg-Landau equation. By 2-dimensional simulation, the comparison of the polarization between samples with and without flexoelectric effect is presented, which shows the importance of considering flexoelectric effect. The flexocoupling coefficients f_{11} and f_{44} shows different effect on domain configuration. Apart from that, the role of the boundary condition and the size effect are also studied.

The work of Shuai Wang is supported by the 'Excellence Initiative' of the German Federal and State Governments and the Graduate School of Computational Engineering at Technische Universität Darmstadt.

[1]P. Zubko, G. Catalan and A.K. Tagantsev, "Flexoelectric effect in solids." Annu. Rev. Mater. Sci., Vol. 43, pp. 387-421, (2013).

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Modeling and Simulation of Electrochemical Cells under Applied Voltage

M. Rossi (TU Dresden, Institute of Solid Mechanics), T. Wallmersperger (TU Dresden, Institute of Solid Mechanics) 15:20

The behavior of an electrochemical thin film under input voltage conditions is numerically investigated. Thin films are present in devices such as micro-batteries and proton-exchange-membrane fuel cells, which are expected to play a significant role in the next generation energy systems for use in vehicles as a replacement to combustion engines [1].

A continuum-based model is developed in order to describe the electrochemical behavior of Nafion membranes (thin films). Diffusive-migrative ionic fluxes and electric field distribution are considered. The fully-coupled electrochemical field is given by the Poisson-Nernst-Planck equations [2]. The model involves initial and interface/boundary conditions appropriate for an electrolytic/galvanic cell. The latter are the Stern layer conditions for polarization effects and the Frumkin-Butler-Volmer equations for electrochemical kinetics of chemical reactions [3, 4]. Time-dependent numerical simulations within a finite element framework are performed.

The results confirm that this model well predicts the behavior of systems, such as redox flow cells or rechargeable batteries, which can either run in electrolytic mode (applied voltage) or in galvanic mode (applied current).

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polymer transducers and its relationship to electromechanical coupling. Journal of Applied Physics. Vol. 101, no. 2, p. 024912, 2007.

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Modeling and simulation of electro-chemo mechanical behavior of ionic polymer-metal composites within the framework of the Theory of Porous Media

S. Serdas (University of Duisburg-Essen), J. Bluhm (University of Duisburg-Essen), J. Schröder (University of Duisburg-Essen) 15:40

Ionic polymer-metal composites serve as electro-mechanical transducers for actuator and sensor applications, see Bar-Cohen [1]. Typically, they are sandwiched between two impermeable electrodes comprising liquid and mobile cations. The actuation mechanism takes place by applying an electric potential (voltage) and the mobile cations move towards the cathode. Due to the relocation of the cations (electrostatic and ionic forces), a deformation of the IPMC can be observed. In contrast, the sensing mechanism is performed by applying a mechanical load yielding to a concentration redistribution and generating an electrical potential inside the IPMC. In Leichsenring et al. [2], the electro-chemical behavior of an IPMC was described within the Theory of Porous Media, see Ehlers [3]. The physical effects under different material compositions by negelecting the motion of the solid and liquid have been investigated in Leichsenring et al. [2]. In the present contribution, the characteristic behavior of an IPMC is described within the framework of TPM by involving the motions of solid and liquid constituents. First, a thermodynamically consistent formulation will be derived and presented. Second, the set of field equations by considering some assumptions will be formulated. And finally, an academic example, cf. Nardinocchi et al. [4], will be provided and discussed.

[1] Y. Bar-Cohen, K.J. Kim, H.R. Choi & J.D.W. Madden: *Electroactive polymer materials.* Smart. Mater. Struct., 16 (2), 2007.

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[3] W. Ehlers: *Foundations of multiphasic and porous materials.*, In Ehlers, W. & Bluhm, J. (eds.), *Porous Media: Theory, Experiments and Numerical Applications.* Springer, 3–86, 2002.

[4] P. Nardinocchi, M. Pezzulla & L. Placidi: *Thermodynamicallly based multiphysic modeling of ionic polymer metal composites.* Journal of Intelligent Material Systems and Structures, 22 (16):1887–1897, 2011.

S 7a : Coupled problems

Thursday 16:30 - 18:30 Marienstr. 13, Ground floor, Lecture hall A
Chair: Detlef Kuhl (Universität Kassel)

Untersuchung des Schließvorgangs von Notfallschützen und ihres Einflusses auf die Strömung von Laufwasserkraftanlagen

C. Seidel (TU Braunschweig, Institut für Statik) 16:30

Verschlussorgane wie Notfallschütze sind bei Wasserkraftanlagen sicherheitsrelevante Bauteile, die bei unvorhergesehenen Ereignissen wie Lastabwurf des Kraftwerks, Blitzschlag, Wellen- oder Getriebebruch sowie anderer Arten von Havarien die Trennung des Volumenstroms zum Kraftwerk bewirken.
Auf Grund der hohen Empfindlichkeit der elektrischen Komponenten eines Kraftwerkes wie z.B. Generatoren oder Umrichter gegen Überdrehzahlen und der daraus resultierenden Wärmeentwicklung in den elektrischen Bauteilen ist es erforderlich, die Notfallschütze in sehr kurzer Zeit zu schließen.
Der Vorgang des schnellen Schützverschlusses löst dabei instationäre Strömungsprozesse wie Schwall- und Sunkerscheinungen aus, deren Intensität mit der Abnahme der Verschlusszeit stark zunimmt. Gleichzeitig besitzen die instationären Strömungsprozesse einen entscheidenden Einfluss auf die Unterströmung des schließenden Notfallschützes, auf den dabei noch abfließenden Volumenstrom und auf die Strömungsgeschwindigkeiten.
Die gekoppelte Interaktion zwischen instationärer Kraftwerksströmung, Schützunterströmung und Schützstruktur wird mit verschiedenen Methoden untersucht und deren Einfluss auf die Kraftwerksströmung, den Schütz, das Kraftwerk und seinen Komponenten sowie dem Kraftwerkskanal bewertet.

Untersuchung von Abstiegsanlagen von Horizontalrechen mit Hilfe von Flachwassergleichungen

L. Ostermann (Institut für Statik, TU Braunschweig), C. Seidel (Institut für Statik, TU Braunschweig) 16:50

Für die strömungsmechanische Optimierung von Wasserkraftanlagen werden experimentelle Untersuchungen und strömungsmechanische Untersuchungen mit Hilfe numerischer Strömungsprogramme auf der Basis von 2D- und 3D-Verfahren eingesetzt.
Für die Errichtung einer Forschungswasserkraftanlage wurde für die numerische Simulation ein Strömungsmodell auf der Basis von Flachwassergleichungen mit Berücksichtigung von Sohl- und Wandreibung mit der Manning-Zahl entwickelt, mit dem sowohl die Kraftwerksströmung als auch der Einfluss der Wasserkraftanlage und ihres Betriebes auf den lokalen Flussabschnitt untersucht werden kann. Für die Diskretisierung der tiefengemittelten Flachwassergleichungen kommt ein Finite-Volumen-Verfahren zum Einsatz, wobei der Flussvektor mit dem HLL-MUSCL-Ansatz berechnet wird und die Zeitintegration mit einem expliziten Verfahren erfolgt. Die Diskretisierung des Berechnungsgebietes erfolgt mit unstrukturierten Dreiecksnetz.

In [1] ist grundsätzlich gezeigt, dass mit Flachwassergleichungsbasierten Verfahren auch strömungsmechanische Optimierungen von Wasserkraftanlagen möglich sind. Im Rahmen der numerische Untersuchung und Optimierung des Kraftwerkstrennpfeilers und der Kraftwerksbuchten wurde auch die im Kraftwerkstrennpfeiler integrierte Abstiegsanlage untersucht und optimiert, da diese einen entscheidenden Einfluss auf die ökologische Durchgängigkeit und auf die Abführung von Treibgut und Sediment besitzt. Eine strömungsmechanisch optimale Form der Abstiegsanlage und ihre richtige Einbindung im Ober- und Unterwasser sind dabei für die Funktionsfähigkeit ebenso wie die optimale Lage des Horizontalrechens, der mit der Abstiegsanlage eine Einheit bildet.
[1] Lars Ostermann, Christian Seidel: 2D und 3D numerische Strömungsanalyse von Kraftwerkstrennpfeilern. Proceedings in Applied Mathematics and Mechanics (PAMM), 2014.

Numerische Untersuchung der Freispiegelströmung in einem Schaufelwasserrad

H. Schippke (TU Braunschweig, Institut für Statik), C. Seidel (TU Braunschweig, Institut für Statik), D. Dinkler (TU Braunschweig, Institut für Statik) 17:10

Im Zuge des Ausbaus der erneuerbaren Energien gewinnt auch in Deutschland die Wasserkraft zukünftig an Bedeutung; besonders im Hinblick auf ihre Grundlastfähigkeit und die netzstabilisierende Wirkung.
Im Gegensatz zu Turbinen als klassische Nutzer der kinetischen Energie, nutzen Wasserräder, mit Ausnahme des Stoßrades, ausschließlich die potentielle Energie des Wassers. Der Vorteil von Wasserrädern besteht in ihrem konstant hohen Wirkungsgradverlauf, der ein großes Jahresarbeitsvermögen ermöglicht, ihrer Robustheit und ihrer hohen ökologischen Verträglichkeit aufgrund der geringen Drehzahlen. Aufgrund dieser Tatsache wurde für die Erschließung der technischen Lücke im Wasserkraftsegment der niederen Fallhöhen und großen Durchflussmengen an der TU Braunschweig die Schlüsseltechnologie der Hochleistungswasserräder entwickelt.
Neben den experimentellen Untersuchungen am Versuchsmodell und den geometrisch-analytischen Verfahren zur Radmodellierung ist ein numerisches Verfahren zur Strömungsanalyse von Schaufelwasserrädern unter Berücksichtigung von freien Oberflächen entwickelt worden. Grundlage des numerischen Modells ist die einheitliche Beschreibung des zweiphasigen Luft-/Wassergebietes mit Hilfe der inkompressiblen Navier-Stokes-Gleichungen in primären Variablen. Die durch das sich drehende Wasserrad sich stetig verändernde Grenzfläche zwischen Struktur- und 2-Phasen-Fluidgebiet wird hierbei im Rahmen der numerischen Berechnung explizit mit Hilfe der SSMUM erfasst, während die implizite Grenzfläche zwischen Luft und Wasser mittels der Level-Set-Methode beschrieben wird.
Ergänzend zu den experimentellen Untersuchungsergebnissen ermöglicht die Analyse der numerischen Berechnungen eine detaillierte Auswertung, selbst an schwer zugänglichen Punkten. Aufgrund der Komplexität der Strömungsvorgänge bei Wasserrädern ist stets ein permanenter Abgleich zwischen Experiment und Numerik erforderlich.

Numerische Strömungsanalyse von Kraftwerkstrennpfeilern unter Verwendung von RANS-Turbulenzmodellen

A. Alfarra (Technische Universität Braunschweig), C. Seidel (TU Braunschweig, Institut für Statik), L. Ostermann (Institut für Statik, TU Braunschweig) 17:30

Bei der Entwicklung von Wasserkraftanlagen ist die numerische Strömungsanalyse ein wichtiges Werkzeug für die Kraftwerksoptimierung. Auf Grund ihrer Effizienz und weitverbreiteten Anwendung im Wasserbau sind hierbei die numerischen Verfahren auf Basis von Flachwassergleichungen von besonderem Interesse.
In [1] wurde das Potenzial solcher Verfahren bei der Optimierung der Strömung um Kraftwerkstrennpfeiler erfolgreich aufgezeigt und Optimierungskriterien herausgearbeitet sowie der Nachweis erbracht, dass die qualitative Formoptimierung mit Flachwassergleichungen möglich ist. Die Frage nach dem Turbulenzeinfluss stellt in diesem Kontext einen interessanten Aspekt dar, weshalb am Beispiel des Kraftwerktrennpfeilers dieser für eine geschlossene Kanalströmung untersucht und mit den Ergebnissen in [1] verglichen wird. Die Unterschiede beider Modellansätze werden herausgearbeitet, der Einfluss der Turbulenz erklärt und die ermittelten Optimierungskriterien hinsichtlich ihrer Gültigkeit auch bei Berücksichtigung der Turbulenz überprüft sowie die durch den Turbulenzeinfluss verursachten Strömungsphänomene aufgezeigt.
Die Modellierung der turbulenten Wasserströmung erfolgt über eine statistische Beschreibung turbulenter Strömungen mittels Reynolds-Gleichungen in Verbindung mit Turbulenzmodellen und bietet im Vergleich zu DNS und LES einen effizienten Ansatz an. Als Turbulenzmodell wird das Standard-k-omega Wilcox Turbulenzmodell verwendet. Die gekoppelten Modellgleichungen aus RANS- und die Transportgleichungen für die Turbulenzgrößen werden mit den zugehörigen Anfangs- und Randbedingungen numerisch im Rahmen einer zeitdiskontinuierlichen Galerkin-Formulierung mit der Raum-Zeit-Finite-Element-Methode diskretisiert und gelöst.
[1] L. Ostermann, C. Seidel: 2D und 3D numerische Strömungsanalyse von Kraftwerkstrennpfeilern. PAMM, 2014.

Optimal Control of a Slot Car Racer

J. Penner (University of Erlangen-Nuremberg), T. Schlögl (University of Erlangen-Nuremberg), S. Leyendecker (University of Erlangen-Nuremberg) 17:50

The primary objective of this work is to present an optimal control method for a mechatronic system and to apply it to compute the time-minimal path for a slot car racer. Here, the used optimal control method and the electromechanically coupled model of a slot car are based on the discretization of the variational description of the system. This method is developed for mechanical systems under the name DMOC (Discrete Mechanics and Optimal Control [4]) and has been extended for mechatronic systems [5, 2].
The task to describe the system dynamics with the discrete variational calculus [3] includes to formulate the electrical, magnetic and mechanical energy of the system [1] and to apply the discrete Lagrange-d'Alembert principle. This is less common in electrical

engineering but leads to a structure preserving time stepping scheme which serves as equality constrains for the nonlinear programming problem, resulting from the discretization of the optimal control problem by the DMOC method. To compute the time-minimal path, the track is described by a piecewise continuously differentiable function and the maximum velocity is prescribed for every section.
Applying the DMOC algorithm generates an offline optimal trajectory, i.e. a sequence of discrete configurations together with a sequence of driving voltages, optimally guiding the system from an initial state to the desired final state. The time-minimal path is achieved by the choice of different cost functions, the sum of time steps, the negative sum of the quadratic momentum and the negative sum of the quadratic velocities. Simulation results show that the momentum formulation yields the lowest number of iterations.
To analyse the system, validate the path function and fit the model parameters, a camera is used to track the vehicle. Furthermore, the tracking allows to compare the motion of the slot car with the optimal trajectory and to correct the vehicle towards the desired state.

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Modal Substructuring of nonlinear plates with geometric nonlinearity

M. Karamooz Mahdiabadi (Lehrstuhl für Angewandte Mechanik, Technische Universität München), D. Rixen (Lehrstuhl für Angewandte Mechanik, Technische Universität München) 18:10

Nonlinear dynamic analysis plays an essential role in the design procedure of machineries encountering large deflections (e.g. Multi-Megawatt Wind Turbines). Besides, it is desirable to have fast and accurate dynamic analysis (e.g. time response) in the design procedure of such nonlinear FE models, which is realizable using model order reduction (MOR) techniques. This work considers model reduction of geometric nonlinear FE models of plate structures. The structure is first divided into small substructures. The

nonlinear reduced order model (NLROM) of each substructure is developed by taking a linear reduced basis in addition to a set of quadratic and cubic nonlinear terms (due to large deflections) with unknown coefficients. The linear basis used in this work for each substructure includes free interface mode in companion with residual flexibility attachment modes. The unknown coefficients of the nonlinear terms are identified by importing a set of forces to the system and determining the underlying displacements (which is called Implicit Condensation and Expansion method). These forces and displacements are then utilized to identify the nonlinear stiffness coefficients of the NLROM in a least square form. Furthermore, the NLROMs will be assembled using the coupling procedure of the Component Mode Synthesis (CMS) method. A typical way to validate the NLROMs is to compute the time integration of some structure's DOFs before reduction and compare them with the corresponding NLROM's DOFs. However, time integration of the primary structure on the one hand is computationally cumbersome. On the other hand, it validates the NLROM for certain load cases and does not guaranty accurate responses for other load scenarios. Accordingly, Nonlinear Normal Modes (NNMs) are proposed as a convergence gauge to overcome the aforementioned drawbacks of time integration comparison. The Applied Force Method (AMF) which is employed in this paper, computes the NNMs of the full model using a few DOFs as well as a wide range of energies where is imposed to the system. A plate structure subjected to large deflections is considered in this study to implement the substructuring method on and validate its NLROM with NNMs. [1] R.J. Kuether, B.J. Deaner, J.J. Hollkamp, and M.S. Allen, Evaluation of Geometrically Nonlinear Reduced Order Models with Nonlinear Normal Modes, AIAA Journal, Vol. 53, No. 11 (2015), pp. 3273-3285. [2] R. Perez, X. Wang, and M. P. Mignolet, "Nonlinear reduced-order models for thermoelastodynamic response of isotropic and functionally graded panels," AIAA Journal, vol. 49, pp. 630-641, 2011. [3] J. J. Hollkamp and R. W. Gordon. Reduced-order models for nonlinear response prediction: Implicit condensation and expansion". In: Journal of Sound and Vibration 318.4-5 (2008), pp. 1139- 1153

S 7a : Coupled problems

Friday 09:00 - 11:00 Marienstr. 13, Ground floor, Lecture hall A
Chair: Stefan Hartmann (Technische Universität Clausthal)

A kinetic energy preserving DG scheme applied to mechanical FSI

S. Ortleb (Universität Kassel) 09:00

The simulation of fluid-structure interaction is highly demanding with respect to each of the involved subproblems, i.e. discretization of fluid and structure equations as well as coupling procedures. In the context of mechanical FSI comprising moving or deforming structures, fluid discretizations need to cope with time-dependent fluid domains and resulting grid deformations in addition to the general challenges regarding e.g. boundary

layers and turbulent phenomena.
Regarding high order discretizations of fluid equations, recent approaches in the simulation of compressible turbulent flow are based on so-called split forms of conservation laws instead of the divergence form in order to guarantee the preservation of secondary physical quantities such as kinetic energy. Conservation of the primary quantities is then achieved by space discretizations with the so-called summation-by-parts property. It has been shown that nodal DG schemes based on Gauss-Lobatto nodes and a lumped mass matrix posses this property. In previous work [1], a kinetic energy preserving(KEP)-DG scheme based on Gauss-Legendre nodes has been constructed based on a generalized summation-by-parts property. This scheme is potentially more accurate and may be also more efficient than its Gauss-Lobatto variant for certain applications. In addition, a better representation of the kinetic energy spectrum in comparison to the non-KEP standard DG scheme has been shown for homogeneous isotropic turbulence.
In this talk, the KEP-DG scheme on Gauss-Legendre nodes is extended to moving fluid grids resulting from an ALE formulation of the fluid equations. Furthermore, first results will be presented for simple test cases regarding mechanical FSI.

[1] S. Ortleb, A kinetic energy preserving DG scheme based on Gauss-Legendre points (2016), to appear in J. Sci. Comput.

Finite Element Approximation of Fluid-Structure Interaction (FSI) Problem with Coupled Wave Propagation

B. Ebna Hai (Helmut Schmidt Universität - Universität der Bundeswehr Hamburg), M. Bause (Helmut Schmidt Universität - Universität der Bundeswehr Hamburg) 09:20

In this contribution, a concept of coupling fluid-structure interaction (FSI) with an ultrasonic wave propagation is proposed, which is referred to as extended Fluid-Structure Interaction (eXFSI) problem. The eXFSI is a one-directional coupling of typical FSI problem with an ultrasonic wave propagation in fluid-solid and their interaction (WpFSI). The WpFSI is a strongly coupled problem of acoustic and elastic wave equations and automatically adopts the boundary and initial condition from previous time step. To the best of our knowledge, such a model is new in the literature. The FSI is modelled in terms of the arbitrary Lagrangian Eulerian (ALE) technique and couples the isothermal, incompressible Navier-Stokes equations with nonlinear elastodynamics using the Saint-Venant Kirchhoff solid model. The WpFSI problems are solved on the moving mesh which is automatically adopted from the FSI problem at each time step. The ALE approach provides a simple, but powerful procedure to couple solid deformations with fluid flows by a monolithic solution algorithm. In such a setting, the fluid equations are transformed to a fixed reference configuration via the ALE mapping. However, combining fluid dynamics with structural analysis traditionally poses a formidable challenge for even the most advanced numerical techniques due to the disconnected, domain-specific nature of analysis tools. The principal aim of this research is the exploration and development of concepts for the efficient numerical solution of the eXFSI problem. The finite element

method is used for the spatial discretization. Temporal discretization is based on finite differences and is formulated as a one step-θ scheme, from which we can consider shifted Crank-Nicolson and the fractional-step-θ schemes. The nonlinear problem is solved by a Newton-like method. Our application of the eXFSI and WpFSI models is the design of on-live and off-live Structural Health Monitoring (SHM) systems for composite material and lightweight structure, respectively. Further applications of the models can be found in biomechanics and biomedicine, e.g. hemodynamics, vibro-mechanics, poroelasticity as well as subsurface and porous media flow. The implementation is accomplished via the software library package DOpElib.

A fully Eulerian approach for fluid-structure interactions with contact

S. Frei (Heidelberg University), T. Richter (Otto-von-Guericke-University of Magdeburg) 09:40

This talk is concerned with the simulation of fluid-structure interaction problems with large solid displacements up to contact of different solids or a solid with a wall. To be able to deal with the topology changes arising in the fluid domain, we use a monolithic fully Eulerian approach.
A monolithic Eulerian approach poses several challenges for a finite element discretisation, as the interface moves over mesh lines and the solution is not smooth across it. If the position of the interface is not considered in the discretisation, severe stability and accuracy issues might arise. In this talk, we present accurate discretisation schemes in space and time as well as a robust numerical framework to circumvent these issues. The basic idea of the discretisation in both space and time is to resolve the interface locally within the discretisation. The spatial discretisation uses a fixed patch mesh independent of the interface location and a local refinement that takes into account the interface. For time discretisation, we develop a time-stepping scheme based on a Galerkin ansatz in time on space-time trajectories that follow the movement of the interface.
Finally, we present simple contact algorithms based on a penalty force and using an active set strategy for the case that no fluid layer remains between the solids and study their influence on the contact dynamics. We apply the numerical framework to the problem of a bouncing ball including the contact with the ground and show numerical results of a ball bouncing down some stairs.

On coupling boundary element and finite element analysis for the efficient simulation of fluid-structure interaction and its application to mold filling processes

M. Harmel, R. Sauer 10:00

Metal casting and polymer molding are widely used for the economical shape processing of complex geometries. In these manufacturing processes, a liquid melt (metal, mineral or synthetic) is filled into a mold with a cavity of the desired shape. Cooling and solidification of the melt results in a product with almost the same shape as the cavity. Numerical simulations can be employed to increase the accuracy of the process. To

this end, several mechanical and thermal phenomena have to be considered: Fluid mechanics within the melt, fluid-structure interaction (FSI) between the melt and its surface, thermomechanical contact between melt and mold, heat conduction within the melt and resulting solidification of the melt.
A new method is presented for creeping mold filling processes. The boundary element method (BEM) and the finite element method are coupled in this work. Under the assumption of low Reynolds numbers, which is valid for creeping flow, the motion of the melt is described by the linear Stokes equations. The transient Stokes equations are solved with the BEM, which only requires boundary discretization. An efficient finite element formulation for liquid membranes is used to model the interaction between melt and mold. Volume discretization is also avoided for the membrane formulation and thus for the entire method. Consequently the computational as well as the meshing effort is highly reduced. The membrane formulation is validated for liquid-solid contact and for FSI problems. It is further investigated in a detailed parameter study for mechanical contact between liquid droplets and rough solid surfaces.
The BEM is also suitable to model heat conduction and (linear) elastic deformations. Therefore solidification of the melt can also be modeled with the BEM.

Keywords: boundary element method, contact mechanics, creeping flow, finite elements, fluid-structure interaction, liquid membranes, mold filling simulation, stokes flow

Two States Analysis for Elastic Solid - Incompressible Liquid Continua in Infinite High Tubes

M. Göttlicher (University of Applied Sciences Erfurt) 10:20

Granular material behaves like a solid in the state of rest. In the state of non convective slow flow [2] it behaves nearly like a solid. The displacements however are not limited similar to a flowing liquid. In the proposed analysis solid and liquid are postulated in the same place. No changes in time are permitted (steady state). The principle of virtual displacements maintains the equilibrium with respect to external loads (specific weight) and boundary conditions [1] separately for the solid part and for the liquid part. The continuity condition is included for the liquid part. Both parts interact by an internal force field. Tension is not permitted. In the state of rest liquid pressure and velocities become zero (mere solid case). In the case of steady state flow (mere liquid case) the displacements become zero. Favorite application for demonstration and derivation is an infinite high plane strain tube [3]. Coulomb friction describes the interaction at the walls. According to St. Venant Hypothesis vertical stress and strain distributions over the cross section are assumed to be constant even if different conditions are given at top and bottom faces. However for the investigation of the performance of the hybrid solid-liquid analysis regarding general applications, top and bottom faces of a slice of finite height are subjected to nonlinear vertical load distributions. In these cases infinity is represented by prescribed constant vertical strain for the solid part and prescribed uniform flow for the liquid part. Nonlinear stress distributions result from nonlinear vertical load distributions acting on the top and bottom faces of the slice. The stresses

consist of a solid part and a liquid part. The relation of both parts follows from the relation of the first stress invariants. The associated displacements and velocities are determined by reduced order approximation of the partial specific weight. Unique forces act on the tube for all possible loads in the permitted range. They are important for the design of containment structures in industry and agriculture. Also the behavior of soil subjected to the forces of foundations of buildings is predictable. Plasticity and other nonlinear investigations may be replaced by the two states analysis of the internally coupled solid-liquid continuum. [1] Reckling, K.A., Gummert, P.: Mechanik, 3rd ed., Springer: Berlin, 2014, p. 686. [2] Zienkiewicz, O.C., Taylor, R.L., Nithiarasu, P.: Finite Element Method for Fluid Dynamics, 7th ed., Butterworth-Heinemann: Oxford, 2013, Chap. 4. [3]Göttlicher, M. Hybrid Solid-Liquid Model for Granular Material, Proceedings 17th IKM, Bauhaus - Universität, Weimar, 2006.

Numerical Study on the fluid-structure interaction in a model aquatic canopy flow

R. Meller (Institut für Strömungsmechanik, Technische Universität Dresden), S. Tschisgale (Institut für Strömungsmechanik, Technische Universität Dresden), J. Fröhlich (Institut für Strömungsmechanik, Technische Universität Dresden) 10:40

This work presents first results from numerical simulations of the flow over aquatic canopies consisting of flexible rectangular blades. The flow is treated in the manner of a Large Eddy Simulation while the blades are described by a geometrically exact Cosserat rod model. To realize the coupling between the fluid and the structures, an Immersed Boundary Method is used. The results obtained with three different Reynolds and Cauchy numbers are compared with experimental data achieving good agreement. The considered range of Cauchy numbers represents three different types of canopies from rigid up to highly flexible plants. The transient flow data and blade positions are statistically analyzed to gain deeper understanding of the complex physical processes in this kind of fluid structure interaction. For example, the correlation of role of large scale motion of the flexible blades in conjunction with coherent vortex structures of the flow is addressed.

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S 7b : Coupled problems

Friday 09:00 - 11:00 Marienstr. 7, 3rd floor, Room 303
Chair: Yousef Heider (RWTH Aachen)

A temperature-based GENERIC approach for the thermodynamically consistent integration of thermoelastic solids

M. Schiebl (Institute of Mechanics, Karlsruhe Institute of Technology), P. Betsch (Institute of Mechanics, Karlsruhe Institute of Technology), C. Hesch (Chair of Computational Mechanics, University of Siegen) 09:00

This work deals with the thermodynamically consistent (TC) time integration of thermoelastic systems with polyconvex energy density functions using the notion of the tensor-cross-product. While energy-momentum preserving integrators are well-known for conservative (isothermal) mechanical systems, Romero introduced in [2, 3] the new class of TC integrators.
While [3] dealt with the sample application of thermo-elastodynamics, the scope of application was extended in [6] to coupled thermo-viscoelastodynamics in temperature form. A first step towards the systematic design of a TC integrator is to cast the evolution equations into the GENERIC (General Equation for Non-Equilibrium Reversible-Irreversible Coupling) framework [1] which reveals additional underlying physical structures of the system. Relying on a polyconvex energy density function and using the notion of the tensor-cross-product [7] we arrive at a polyconvex version of the GENERIC framework. Further applying the notion of a discrete gradient leads to a TC integrator.
Using the entropy as the thermodynamical state variable as in [3, 4] the GENERIC framework possesses an easy structure. However, this choice of thermodynamical state variable only allows to prescribe entropy Dirichlet boundary conditions directly. This drawback can be compensated by using Lagrange-multipliers to be able to handle temperature Dirichlet boundary conditions leading to an extended system of algebraic equations to be solved, see [4]. Alternatively, the present work uses the temperature as the thermodynamical state variable, see also [5, 6]. The presentation includes several simulations with different boundary conditions and an energy-based termination criterion.

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[7] J. Bonet, A. J. Gil, and R. Ortigosa. On a tensor cross product based formulation of large strain solid mechanics. *International Journal of Solids and Structures*, 84:49–63, 2016.

Identification of damages using inverse analysis in 3D coupled thermo-hydro-mechanical problems

L. Nguyen-Tuan (Bauhaus-Universität Weimar), C. Koenke (Bauhaus-Universität Weimar), T. Lahmer (Bauhaus-Universität Weimar) 09:20

Many masonry dams were built at the beginning of the twentieth century, e.g., the Fürwigge and Ennepe Dams in Germany, or the Theodore Roosevelt Dam in Arizona, USA. Material properties of these masonry dams may have remarkably changed due to aging, weathering and chemical effects. Consequently, some critical damage zones or cracks could be present. Generally, in damaged regions the properties of the material (e.g. stiffness, permeability, porosity and thermal conductivity) change visibly. For such situations it is more useful and economic, when the damage is directly identified by evaluating the measurement data from the sensors installed in the dams, e.g., during the impounding period instead of performing time intensive and costly experiments. In this contribution, we propose a method to localize damages and determine the degree of the damage using inverse analyses. As measurement data, transient displacements, temperatures and water pressures are used. The damage itself is described by a finite number of parameters. The inverse problems are solved by global nonlinear optimization algorithms. These methods are applied for the identification of the damage in the Füwigge masonry dam based on a three dimensional non-linear coupled thermo-hydro-mechanical problem [1]. The effects of uncertainties in the measurements, the size and degree of the damage on the accuracy of the solutions are also considered in the contribution.

[1] Nguyen-Tuan, L., Koenke, C., Bettzieche, V. and Lahmer, T. “Numerical modeling and validation for 3D coupled-nonlinear thermo-hydro-mechanical problems in masonry dams.” Computers and Structures (2017) Vol.178, 143-154

Description of the Damage and Healing Behavior of an Extrinsic and Autonomous Self-Healing Anisotropic Material

J. Bluhm (University of Duisburg-Essen), S. Specht (University of Duisburg-Essen), J. Schröder (University of Duisburg-Essen) 09:40

Polymers and polymeric composites are used in a wide range of technical applications, e.g. for wind turbine blades or aerospace applications. But failures, which often results

from the propagation of microdamages inside the structure are hard to detect and to repair [1]. In many cases the only way is to replace the damaged part. This can be very difficult and costly for example in case of off-shore wind turbines.

In order to extend the lifetime of such structural parts, Self-healing materials can be used. These materials have the ability to repair autonomously microdamages, see [2]. If a crack breaks through such a microcapsule, which is filled with liquid healing agents (monomer), the liquid flows into the crack due to capillary action. After contact between the healing agents and the dispersed catalysts, the monomer polymerizes and the crack is healed.

For the simulation of such a multiphasic material, the Theory of Porous Media is used in this contribution [3, 4]. The multiphase system consist of the polymeric matrix material, in this matrix dispersed catalysts, air, liquid polymer as healing agents and polymerized healed material. Damage is considered by a continuum damage mechanics model and healing is described by a phase transition from the liquid polymer to the polymerized healed material [5]. In order to simulate self-healing composites, anisotropy will be considered within the model.

At the end, the results of different micro- and macroscopic boundary value problems will be shown in order to demonstrate the applicability of the developed model.

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A thermomechanical analysis of interfaces between the mating parts in ultrasonic wire bonding

S. Mostafavi (RWTH-Aachen University), Y. Heider (RWTH Aachen), B. Markert (RWTH Aachen University) 10:00

Ultrasonic welding (USW) is an alternative solution for bonding process especially in automotive industry. As an alternative for crimping technology in wire bonding, ultrasonic welding is applied in order to create solid state joints between the mating

parts at low temperature and low energy consumption compared to other common welding processes, such as oxy-fuel welding and arc welding. Ultrasonic welding of metals is a joining technique as a combination of applying pressure and frictional vibrations within the range of ultrasonic frequencies. Thermo-structural analysis of ultrasonic wire bonding has been performed by means of the 3D finite element method by Ding and Kim [1]. Thermomechanical analyses of ultrasonic welding of aluminum alloy have been performed by Siddiq and Ghassemieh [2].
The present work presents a thermomechanical analysis of the interface between two mating parts in USW. For this reason, temperature distribution at bonding place due to frictional vibrations and pressure is investigated with the finite element method. Microsections obtained during experimental investigations done in previous studies show the softening of aluminum strands at some bonding parts within the investigated wire bundle [3]. The obvious difference in microsections from different welding samples, which can be interpreted as different local temperature rises, was the motivation for this study to further investigate the thermomechanical aspects of the USW by use of FEM simulations.

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[2] Siddiq, A., Ghassemieh, E.: *Thermomechanical analyses of ultrasonic welding process using thermal and acoustic softening effects.*, Mech. Mater. 40:982-1000 (2008).

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Model order reduction for thermomechanical problems including radiation

S. Rother (TU Dresden, Institute of Solid Mechanics), M. Beitelschmidt (TU Dresden, Institute of Solid Mechanics) 10:20

Transient thermal simulations often correspond with long computation times, especially when parameter studies are performed. Model order reduction allows to overcome this difficulty. If thermal radiation has to be considered, the problem is nonlinear and the Krylov subspace method cannot be applied directly. Defining radiation as external load provides the opportunity to evade this. Therefore, the system is split into one part for the computation of the radiation heat fluxes and one for the temperature field, which can be solved iteratively. Thermal loads like convection and radiation are distributed over the whole surface resulting in a high number of inputs and outputs. This limits the reduced dimension since it is a multiple of this number. Hence, input reduction is required. Here, the most challenging part is to determine the columns of the input matrix in a way that the load vectors, which occur during simulation, are linear combinations of these input vectors. Simultaneously changing loads, e.g. nodes having the same temperature, heat flux or convection boundary condition, are grouped into one column of the input matrix.

However, this is not reasonable for radiation since here the heat fluxes depend on the actual temperatures. For finite elements with quadratic shape functions a first reduction is performed with element surfaces instead of nodes as inputs. So, the size of the input matrix can be reduced by a factor of three without any loss of accuracy. Using the load vectors from one transient simulation as input vectors has proven as most efficient for further reduction to a very small number of inputs. Afterwards, parameter studies can be performed yielding good results within a broad parameter range. The corresponding thermal stresses, which are assumed to be quasi-static, can be obtained at distinct critical points directly from the displacements at the master nodes of a Guyan reduced model even if the thermal loads are changing.

Thermo-mechanical modeling of turbine blades taking into account structural defects

A. Kunin (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), S. Löhnert (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 10:40

In turbine blades of aero-engines typical defects are cracks in the range of several centimeters down to 40-70 microns. In addition to the high centrifugal forces, the temperature near the surface can reach up to 1000°C.

To accurately simulate 3D crack propagation in an inelastically and thermo-mechanically behaving material leads to an extensive numerical effort. Therefore, the extended finite element method (XFEM)[1] is widely used for simulations of fracture mechanics problems considering cracks directly at the element level. Discontinuities in the displacement and temperature field[2] are allowed and simultaneously the crack opening displacement and crack tip stress field are reproduced accurately with the XFEM.

Since crack closing and non-physical penetration of the crack surfaces may occur at element level under certain load conditions, it becomes necessary to enforce the non-penetration condition (for crack surfaces) like in multi body systems with contact. Additionally, pressure depended heat conduction across crack surfaces should be taken into account for thermo-mechanically coupled problems which are investigated in this work. The proposed contact formulation is embedded in an XFEM framework based on the work by Mueller-Hoeppe et al.[3]. Only normal contact conditions are implemented. The node-to-segment approach proposed in [3] is extended to ten-node tetrahedral elements with quadratic shape functions.

The penalty method is used to enforce the constraint equations for the displacements avoiding unphysical penetration of the crack surfaces. Results of mechanical and thermo-mechanical benchmark tests achieved by the developed extended finite element formulation including normal contact and pressure depended heat conduction are presented.

[1] N.Sukumar, N. Moes, B. Moran, T. Belytchko; “Extended finite element method for three-dimensional crack modeling”, Int. Journal for Numerical Methods in Engineering, 2000

[2] M. Duflot, “The extended finite element method in thermoelastic fracture mechan-

ics",Int. Journal for Numerical Methods in Engineering, 2008
[3] Mueller-Hoeppe D.S., Wriggers P., Loehnert S.; "Crack face contact for a hexahedral-based XFEM formulation", Comput Mech (2012) 49:725-734

S 7a : Coupled problems

Friday 11:30 - 13:30 Marienstr. 13, Ground floor, Lecture hall A
Chair: Anne Jung (Universität des Saarlandes)
Stefan Diebels (Universität des Saarlandes)

A Variational Homogenization Approach on Large Strain Micro-Electro-Mechanics

D. Vallicotti (University of Stuttgart), A. Sridhar (Institute of Applied Mechanics (CE)), M. Keip (University of Stuttgart) 11:30

Functional materials have received a lot of attention in recent years. Composite materials of soft polymers embedded with ferroelectric particles are advantageous due to the large deformations possible in such materials. Phenomenological modeling of this electromechanical coupling phenomena has been extensively covered, however complex multi-scale interactions based on a microscopic electric domain evolution and its effect on the overall macroscopic response is of utter importance for a understanding of the underlying physical phenomenon. This necessitates the use of multi-scale approaches such as computational homogenization to reliably predict and in turn enhance the overall material response.
We propose a *variational framework for micro-electro-mechanical response at large deformations* embedded into a scale-bridging scenario by using *homogenization techniques* in order to define the macroscopic overall response of electro-active materials. Starting point is a *rate-type saddle point variational principle on the microscale* yielding the Euler-Lagrange equations and a Ginzburg-Landau-type evolution equation for the polarization order parameter. A challenge is to link the gradient-type continuum description of the microstructure to a local electro-mechanical macro-continuum. This is achieved by exploiting a generalized Hill-Mandel macro-homogeneity condition, yielding periodic boundary conditions at the faces of the microstructure.
Numerical examples demonstrate the capabilities of the framework and show the effect of particle interactions based on evolving electric domains on the overall macroscopic response.

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2. A. Sridhar, M.-A. Keip, C. Miehe, *Homogenization in Micro-Magneto-Mechanics*, Computational Mechanics, 58, 151–169, 2016.

3. C. Miehe, D. Vallicotti, S. Teichtmeister, *Homogenization and multiscale stability analysis in finite magneto-electro-elasticity. Application to soft matter EE, ME and MEE composites*, Computer Methods in Applied Mechanics and Engineering, 300, 294–346, 2016.

Coupled contact problems in piezoelectricity

J. Gwinner 11:50

In this contribution we are concerned with unilateral contact problems with friction in piezoelectricity.
First we extend the mathematical modelling and solvability analysis given in [1] for linear transmission problems for piezoelectric elastic materials to this class of nonlinear free boundary value problems. Similar to [2] for micropolar hemitropic elasticity, we apply potential methods which transform the weak formation of these contact problems to boundary variational inequalities involving boundary integral operators. Based on our boundary variational inequality approach we prove existence and uniqueness theorems for weak solutions. We prove that the solutions continuously depend on the data of the original problem and on the friction coefficient. We treat also the case when the body is not fixed, but only submitted to some forces along some part of the boundary and is in unilateral frictional contact with a rigid foundation. In this situation we present necessary and sufficient conditions of solvability.
Then we study the numerical approximation of these coupled contact problems. In virtue of our boundary variational inequality approach we can reduce the spatial dimension and employ finite element discretization on the boundary, only, what leads to the numerical treatment by the well-known boundary element method (BEM). Since we here admit approximations of higher order, we are confronted with nonconforming approximation. To this end we extend the numerical analysis given in [3] for a scalar model problem to the full vector case of coupled piezoelectricity.
[1] T. Buchukuri, O. Chkadua, D. Natroshvili, A.-M. Sändig, Solvability and regularity results to boundary-transmission problems for metallic and piezoelectric elastic materials, Math. Nachr., Vol. 282, 1079 - 1110 (2009).
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[3] J. Gwinner, On the p-version approximation in the boundary element method for a variational inequality of the second kind modelling unilateral contact and given friction, Appl. Numer. Math., Vol. 59, 2774 - 2784 (2009).

Modeling and simulation of magnetorheological elastomers: a comparison of continuum and dipole approaches

P. Metsch (TU Dresden), D. Romeis (Leibniz-Institut für Polymerforschung e.V.), M. Saphiannikova (Leibniz-Institut für Polymerforschung e.V.), M. Kästner (TU Dresden) 12:10

Magnetorheological elastomers (MREs) represent a class of composite materials that consist of micron-sized magnetizable particles which are embedded into a non-magnetizable polymer matrix. Due to mutual interactions of the particles, MREs are able to alter their effective material behavior reversibly if subjected to an external magnetic field. Moreover, they show a large magnetostrictive response: compared to pure ferromagnetic materials, their field-induced deformation is increased by orders of magnitude. Since the effective material behavior of MREs is essentially determined by the constitutive properties of the individual components and their geometrical arrangement within the composite, this contribution will apply a microscopic modeling approach for the coupled magneto-mechanical problem. Starting from the properties of the magnetizable particles and the elastomer matrix, a model based on a continuum formulation of the problem is presented.
In the literature different theoretical models have been proposed to describe the properties of MREs. Nevertheless, the predictions of available models often vary significantly since they are based on different assumptions and approximations. Up to now the actual accuracy and the limits of applicability are widely unknown. In the present work, the results of the microscale continuum and a dipolar mean field approach are compared with regard to their predictions for the magnetostrictive response of MREs. To this end, different isotropic samples with varying particle volume fractions are considered. A sample averaging process for each particle volume fraction ensures the validity of our findings.
It turns out that there is a very good agreement between both modeling strategies, especially for entirely random microstructures. In contrast, a comparison of the finite element results with a modified approach, which – similar to the continuum model – is based on calculations with discrete particle distributions, reveals clear deviations. Our systematic analysis of the differences shows in how far the dipolar mean field approach is superior to other dipole models.
Acknowledgements:

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Leakage currents in nanogenerator concepts examined with phase field simulation

F. Wöhler, I. Münch (KIT), W. Wagner (Karlsruher Institut für Technologie) 12:30

For the purpose of energy harvesting on the nanoscale with ferroelectric barium titanate (BTO), the presented nanogenerator concept intends to transform parasitic mechanical oscillation into usable electric energy. Difficulties in experiments occur in sample preparation and measurements of ferroelectric properties and also in analysing generator characteristics, in particular the effect of leakage current. Therefore, simulations on the basis of a finite element phase field model are used to predict experimental results. Within the performed simulations, the evolution of domain topology is examined and expected

leakage current displayed. Hereby, leakage is implemented in different phenomenological approaches.
First, Ohm's law represents a linear relation between leakage current and the electric field, and leads to reasonable results for one and higher dimensional models. On the other hand, for the space charge limited current relation (SCLC), which has a quadratic dependency on the electric field, it is observed that for one dimensional problems the current flow is suitable, but for higher dimensional problems SCLC is only indicated in positive axis directions independent of current initiation. Therefore, a new leakage current equation building upon a quadratic relation to the electric field is discussed for feasibility.

FEM-analysis of multiferroic nanocomposite: Comparison of experimental data and numerical simulation

V. Lemke (Universität Duisburg-Essen), M. Labusch, J. Schröder (Universität Duisburg-Essen), H. Wende 12:50

The combination of electric and magnetic materials opens new possibilities in the field of sensor technologies and dara storage [1]. These magneto-electric (ME) materials have the property to change a physical ferroic quantity into another, i.e. a magnetic field can change the electric polarization. The combination of multiple ferroic characteristics within materials is also called multiferroic. Since magneto-electric single-phase materials have a synergy of the polarization and magnetization at very low temperature, they are not favorable in technical applications. However, ME composites, consisting of ferroelectric and ferromagnetic phases, produce a strain-induced magneto-electric product property at room temperature [2]. In these composites, two different effects can be differentiated, the direct and the converse ME effect. The first one describes a polarization which is magnetically caused. In detail, a magnetic field is applied which produces a deformation of the magneto-active phase and in turn it is transferred to the electric-active phase. Therefore, one can discover a strain-induced polarization. The second effect to observe is a magnetization caused by an electric field. In our contribution, we focus on a (1-3) composite, where cobalt ferrite nanopillars are embedded in a barium titanate matrix based on the experiments described in [3]. In the numerical simulations we compare the changes of the strain-induced inplane polarizations of the ferroelectric matrix with experimental measurement results. Furthermore, we take a closer look on the magneto-electric coupling coefficient.

[1] N. A. Spalding and M. Fiebig, The renaissance of magnetoelectric multiferroics. *Materials Science*, 309, 391–392, 2005.

[2] J. van Suchtelen, Product properties: a new application of composite materials. *Philips Research Reports*, 27, 28–37, 1972.

[3] C. Schmitz-Antoniak, D. Schmitz, P. Borisov, F. de Groot, S. Stienen, A. Warland, B. Krumme, R. Feyerherm, E. Dudzik, W. Kleemann and H. Wende, Electric in-plane polarization in multiferroic $CoFe_2O_4/BaTiO_3$ nanocomposite tuned by magnetic fields. *nature communications*, 4, 1–8, 2013.

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Heat Conduction in a Phase Field Model for Martensitic Transformation

S. Schmidt (TU Kaiserslautern), R. Müller (TU Kaiserslautern) 13:10

The overall material properties usually depend on the microstructure. Iron for instance, is an allotrope featuring different crystal orientation variants. A martensitic phase is usually desired in near surface regions, rendering the workpiece more resistant to mechanical wear. The process of cryogenic turning aims at causing a martensitic tranformation, where the temperature field is in general dependent on space and time [1]. We study the martensitic transformation with a phase field model, where we consider the Bain transformation path in a small strain setting. For the order parameter, interpolating between an austenitic parent phase and martensitic phases, we use a Ginzburg-Landau evolution equation, assuming a constant mobility. In [2], a temperature dependent separation potential is introduced. We use this potential to extend the model in [3], by considering a transient temperature field, where the temperature is introduced as an additional degree of freedom. This leads to a coupling of both the evolution equation of the order parameter and the mechanical field equations (in terms of thermal expansion) with the heat equation. The model is implemented in FEAP as a 4-node element with bi-linear shape functions. Numerical examples are given to illustrate the influence of the temperature on the evolution of the martensitic phase.

[1] Steven Becker, Patrick Mayer, Benjamin Kirsch, Jan C. Aurich, Erik v. Harbou, and Ralf Müller. Transient finite element simulation of the temperature field during cryogenic turning of metastable austenitic steel aisi 347. *PAMM*, 16(1):303–304, 2016.

[2] Simon Schmidt, Carolin Plate, Regina Müller, Ralf Müller, Jerome Meiser, and Herbert M. Urbassek. A phase field model for martensitic transformations with a temperature-dependent separation potential. *PAMM*, 16(1):481–482, 2016.

[3] Regina Schmitt, Ralf Müller, Charlotte Kuhn, and Herbert M. Urbassek. A phase field approach for multivariant martensitic transformations of stable and metastable phases. *Archive of Applied Mechanics*, 83(6):849–859, 2013.

S 7b : Coupled problems

Friday 11:30 - 13:30 Marienstr. 7, 3rd floor, Room 303
Chair: Sigrun Ortleb (Universität Kassel)

Nonintrusive Cosimulation Schemes

T. Moshagen (TU Braunschweig) 11:30

In engineering, it is a common desire to couple existing simulation tools together into one big system by passing information from subsystems as parameters into the subsystems under influence. As executed at fixed time points, this data exchange gives the global method a strong explicite component, and as flows of conserved quantities are passed across subsystem boundaries, it is not ensured that systemwide balances are fulfilled: the system is not solved as one single equation system. These *balance errors* can accumulate and make simulation results inaccurate. Use of higher-order extrapolation in exchanged data can reduce this problem but cannot solve it. The remaining balance error has been handled in past with balance correction methods which compensate these errors by adding corrections for the balances to the signal in next coupling time step. This gives rise to the problem that establishing balance of one quantity *a posteriori* in general disturbs the balances of quantities that depend on the exchanged quantities, usually energy. In this work, a method is suggested which allows to choose the quantity that should be balanced freely, thus providing stability.
A convergence proof is given for cosimulation schemes with and without balance correction.

Finite-element-based simulation of multi-physics materials

M. Schenke (Universtät Stuttgart - GSaME), W. Ehlers (University of Stuttgart) 11:50

Many natural and engineered substances can be assigned to the class of multi-physics materials. Therein, their macroscopically observed behaviour is governed by different micro-structural physical phenomena. For instance, when electro-active polymers (EAP) are subjected to an electric field, the resulting chemical and electrical imbalances trigger micro-structural diffusion processes which reestablish the equilibrium state, thereby causing macroscopic deformations. Further examples for these materials are partially or fully saturated porous media (e. g. foams, soils, filters, fibre-reinforced plastics), chemical- or electrical-active materials (e. g. hydrogels, lithium-ion batteries) or biological tissues (e. g. bone, cartilage). Addressing the simulation of multi-physics materials, which often exhibit a complex and heterogeneous micro-structure, it is more convenient to proceed from a macroscopic modelling approach. For this purpose, the macroscopic Theory of Porous Media (TPM) is chosen as a suitable modelling framework. The material models, which are usually developed during either academic or industrial research projects, are often implemented into self-developed programme codes to scrutinise the advancements and but also the limitations of the material models. However,

these codes often lack the necessary functionality, for instance, in terms of modelling features necessary for building complex initial-boundary-value problems (IBVP) and user interaction, to be used within the scope of industrial applications.
In this regard, the present contribution bridges the gap between research and industrial application. In particular, it addresses a general interface between the research code PANDAS, which is a finite-element (FE) solver especially designed for the efficient solution of volume-coupled multi-field problems, and the commercial FE packages Abaqus and LS-DYNA. In both cases, the coupling is based on the user-defined element subroutines of Abaqus and LS-DYNA, respectively. This procedure allows, on the one hand, a straight-forward embedding of all material models of PANDAS into commercial FE packages. On the other hand, it provides, in comparison with the native user-defined subroutines, a user-friendly programming environment for user-defined material models with an arbitrary number of degrees of freedom. Furthermore, the coupling allows for the parallel analysis of large-scale problems on high-performance computing clusters. The capabilities of the coupling procedures are illustrated by the simulation of various coupled multi-field problems, such as partially or fully saturated soils, vacuum-assisted resin injections (VARI) of dry fibre fabrics or chemically or electro-chemically driven swelling phenomena as they appear, for example, within hydrogels.

The Segment to Segment Penalty Coupling Approach for Rolling Contact Simulations

T. Palanichamy (Institute of Mechanics and Computational Mechanics), 12:10
U. Nackenhorst (Institute of Mechanics and Computational Mechanics),
A. Suwannachit (Continental AG)

The Arbitrary Lagrangian Eulerian (ALE) kinematics framework is used widely in rolling contact analysis due to its main advantages in implementing the detailed contact analysis with local mesh refinement and time independent formulation of elastic stationary rolling [1]. Tires with circumferential grooves satisfy the axisymmetric constraint whereas tires with detailed tread pattern do not comply with axisymmetric constraint of the ALE formulation. The goal of this research is to develop the coupling of tread pattern (transient dynamic Lagrangian) with tire body (steady state ALE) using kinematic constraints. The advantage of such coupling will complete the whole picture of treaded tires simulation in ALE framework.

In this article, two test cases are proposed in fully Lagrangian framework, one for developing the coupling constraints and the other one to implement a deformable - deformable contact discretization using segment to segment penalty approach.

The first test case is a deformable - rigid formulation and the coupling constraints are added to the weak form as given in [3]

$$G_M(\delta\boldsymbol{u},\boldsymbol{u}) = \int_{B_o} \rho_o \ddot{\boldsymbol{u}}\cdot\delta\boldsymbol{u}\, dV + \int_{B_o} \boldsymbol{S} : \boldsymbol{\delta E}\, dV - \int_{\partial_t B_o} \bar{\boldsymbol{T}}\cdot\delta\boldsymbol{u}\, dA + \int_{\partial_c \Phi(B_o)} (\boldsymbol{\tau}^{\alpha}\delta\boldsymbol{s}_{\alpha} + p\delta d_N)\, da = 0\,. \tag{6.4}$$

The second test case is about the coupling of two non conformal mesh. Here the two flexible

bodies are discretized using segment to segment penalty approach as formulated in [3]. The contact patch test is done to exhibit its robustness.

Now the next step would be coupling of ALE relative kinematic framework with Lagrangian framework. From [2], the enforcement of stick condition by slip velocities does not agree with analytical solutions and a novel approach for the stick condition in ALE framework by penalizing the slip distance is introduced.This approach which has been shown for a deformable-rigid road contact will be extended to deformable-deformable formulation(ALE tire structure and Lagrangian tread block). The slip velocity $\dot{s}_{h\alpha}$ which comes from the convective particle velocity and the translatory tread block velocity is equated with ALE description of slip velocity under steady state condition as given below.

$$\int_{\partial_c \Phi(B)} \delta\dot{\boldsymbol{s}} \cdot (Grad\ \boldsymbol{s} \cdot \boldsymbol{w}) = \int_{\partial_c \Phi(B)} \delta\dot{\boldsymbol{s}} \cdot \dot{s}_{h\alpha} \boldsymbol{a}_\alpha\ da \tag{6.5}$$

Linearizing the above term with respect to displacement and slip variables and after that with the FE discretization of global displacement field and the spatial slip variables, a coupled linearized problem as given in [2] can be obtained.Within a monolithic scheme, the coupled linearized problem is solved for slip variables and then the coupling constraints are implemented for two flexible bodies as discussed in above two test cases.

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Metal Particle Melting for Powder Based Additive Manufacturing Using Optimal Transportation Meshfree Method

H. Wessels (Leibniz Universität Hannover, Institut für Kontinuumsmechanik), C. Weißenfels (Leibniz Universität Hannover), P. Wriggers (Leibniz Universität Hannover, Institut für Kontinuumsmechanik) 12:30

Selective Laser Melting (SLM) is an additive manufacturing (AM) process, where a powder bed is partially melted. Layer by layer, complex three dimensional geometries including overhangs can be produced, because non-melted powder acts as support structure.

Up to date the multiple interacting physical phenomena are not yet fully understood. This is why the material and process development mainly relies on experimental studies that are time and cost intensive. Novel simulation tools such as meshless methods offer the potential to gain a deeper understanding of the process - structure - property interaction. This can help to find optimal process parameters and to individualize AM

manufactured parts by locally altering material properties.

Using conventional FEM methods, extremely large deformations of the mesh lead to ill-shaped elements and per consequence to degenerate computations. Meshfree methods eliminate the mesh dependency by employing a more flexible formulation to relate a point of integration to its neighboring nodal points. This requires flexible shape functions that depend on the nodal positions only [1].
The Optimal Transportation Meshfree (OTM) Method is a meshless method based on the weak formulation of the differential equations and can be downscaled to the Finite Element Method. It accounts for a broad variety of materials ranging from solids to fluids [2] including thermo-mechanical behavior.
This flexibility makes the OTM an optimal tool to simulate the melting of powder particles and the motion of the melt flow. An approach to account for the phase transition and the fusion of particles using OTM will be presented.

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[2] Li, B, Habbal, F, Ortiz, M. Optimal transportation meshfree approximation schemes for fluid and plastic flow. *International Journal for Numerical Methods in Engineering 2010.* 83(12):1541-1579

Mixed variational formulations for multi-field problems

M. Dittmann (Universität Siegen), C. Hesch (Universität Siegen), M. Franke (Karlsruher Institut für Technologie (KIT)) 12:50

In the present contribution we focus on novel computational formulations for multi-field coupling in large strain problems. In particular, polyconvex large strain thermoelasticity as well as polyconvex large strain phase-field fracture formulations are considered.
The formulations of both multi-field problems are based on an extended kinematic set, the deformation gradient (line map), its co-factor (area map) and its determinant (volume map), and their conjugate stresses. The strain measures are defined via the tensor cross product between second order tensors as proposed in Bonet et al. [1]. Thereby, the linearization of the systems can be expressed in compact form and the conjugate stresses relate to classical stress tensors in elegant manner. Moreover, the formulations allow for the introduction of mixed variational principles in a straightforward manner.
For the thermomechanical system, a Hellinger-Reissner type variational principle based on the definition of a complementary energy density function is applied. Therein, the deformed geometry and the absolute temperature as primal variables are supplemented by the newly introduced conjugate stresses. The thermomechanical coupling is directly implemented between the temperature and the conjugate stress to the Jacobian determinant, see Dittmann [2].

Variationally consistent formulated phase-field methods to fracture are able to predict complex three-dimensional crack patterns. Here, we propose a novel approach based on a mixed Hu-Washizu formulation, where the primal variables are given by the deformed geometry, the extended set of strains and conjugate stresses as well as the phase-field variable, see Hesch et al. [3].
This promising approaches enable great flexibility and clarity for the development of new multi-field formulations, since the constitutive laws can be solved as separate field. This can be done without enlarging the system to be solved using suitable static condensation procedures, hence, no additional computational effort for the solution is required. To this end, we apply discontinues constant and linear interpolations to the stresses and/or strains, whereas the displacement field and the additional field of the corresponding multi-field problem is discretized ultilizing quadratic B-spline based shape functions. The chosen approximations ensure optimal convergence.

[1] Bonet, J., Gil, A.J. and Ortigosa, R. *A computational framework for polyconvex large strain elasticity*. Comput. Methods Appl. Mech. Engrg., 283:1061–1094, (2015).

[2] Dittmann, M. *Isogeometric analysis and hierarchical refinement for multi-field contact problems*. PhD thesis, University of Siegen, (2016).

[3] Hesch, C., Gil, A.J., Ortigosa, R., Dittmann, M., Bilgen, C., Betsch, C., Franke, M., Janz, A. and Weinberg, K. *A framework for polyconvex large strain phase-field methods to fracture*. Comput. Methods Appl. Mech. Engrg., (2016), submitted.

S 8: Multiscales and homogenization

Organizers: Bernhard Eidel (Universität Siegen)
Stefan Löhnert (Leibniz Universität Hannover, Institut für Kontinuumsmechanik)

S 8 : Multiscales and homogenization

Tuesday 14:00 - 16:00 Marienstr. 7, 3rd floor, Room 303
Chair: Rolf Mahnken (Universität Paderborn)

An Algorithmically Consistent Approach for Computing the Macroscopic Tangent in FFT-based Homogenization

F. Göküzüm (University of Stuttgart), M. Keip (University of Stuttgart) 14:00

Lately, the FFT-based method suggested by Moulinec & Suquet [1] for the homogenization of complex composites has increased in popularity due to its high computational speed [5]. The present work gives a computational framework for evaluating the consistent tangent for FFT-based homogenization. It is inspired by the works on multiscale

FE [2] and multiscale FE-FFT methods [3, 4]. The proposed consistent tangent for FFT-based approaches offers an alternative to numerical tangents calculation, which are carried out by calculating a corresponding number of load steps. Especially in the context of multi-scale methods, e.g. FE^2 or FE-FFT, the computation of a consistent macroscopic tangent is crucial. Computing the tangent numerically can be costly with respect to computational time, especially for nonlinear problems. We will show that the use of an algorithmic tangent offers a more efficient and faster calculation of the macroscopic tangent, as its governing equations are all linear with respect its primary variables. The viability of the method holds for linear as well as for nonlinear material behaviour, including viscoelasticity and nonlinear elasticity.

[1] H. Moulinec, P. Suquet: A fast numerical method for computing the linear and nonlinear mechanical properties of composites, *Académie des Sciences*, 2, 1417–1423 (1994).

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Homogenization of periodic microstructures with FFT-based higher order schmes

F. Dietrich (TU Kaiserslautern), D. Merkert (TU Kaiserslautern) 14:20

In 1994, Moulinec and Suquet [1] presented a new homogenization method for periodic microstructures, such as composites, based on the Fast Fourier Transform (FFT), which allows to directly analyse data on a given structured grid, e.g. as it arises in microtomography.
Using this algorithm, called the *basic scheme*, Tran, Monchiet and Bonnet [2] developed an extended homogenization framework, making it possible to include macroscopic gradients and effects of arbitrary high derivatives into the microscopic analysis.
During the presentation, we want to shortly present the general idea and the main tools needed in the basic scheme and its higher-order variant on the basis of linear elasticity.

To be more precise, writing the equations of classic linear elasticity as an asymptotic expansion series, we will derive a more general form of the cell problem by means of scale separation. The solution of the resulting *Lippmann-Schwinger-type equation*

$$\left[\mathrm{Id} + \Gamma^0 * (C - C^0)\right] \tilde{\epsilon} = -\Gamma^0 * p^\alpha + \theta^\alpha$$

is then given by the zero-mean strain tensor $\tilde{\epsilon}$ that can be determined by CG-methods, as it was shown in [3]. Here, Id denotes the identity operator, C is the stiffness tensor containing elastic coefficients of the material, C^0 represents a reference material, Γ^0 is the Green operator connected to C^0, p^α and θ^α are additional terms depending on the order α of the problem and the asterisk denotes the convolution.
Moreover, we want to outline how one could combine the idea of higher-order terms with other existing methods, such as the polarization scheme [4] or multiscale models [5].

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A fast numerical method for computing the linear and nonlinear properties of composites. *Comptes Rendus de l'Académie des Sciences Paris II 318 (1994): 1417–1423*

[2] T. Tran, V. Monchiet, G. Bonnet.
A micromechanics-based approach for the derivation of constitutive elastic coefficients of strain-gradient media. *International Journal of Solids and Structures 49 (2012): 783-792*

[3] J. Vondřejc, J. Zeman, I. Marek.
An FFT-based Galerkin method for homogenization of periodic media. *Computers and Mathematics with Applications 68 (2014): 156-173*

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A polarization-based FFT iterative scheme for computing the effective properties of elastic composites with arbitrary contrast. *International Journal for Numerical Methods in Engineering 89 (2012): 1419-1436*

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A multiscale approach for modelling progressive damage of composite materials using fast Fourier transforms. *Computer Methods in Applied Mechanics and Engineering 268 (2014): 871-883*

Fourier-accelerated computational homogenization based on a finite element formulation

M. Leuschner (University of Stuttgart), F. Fritzen (University of Stuttgart) 14:40

Computational homogenization methods are used to analyze heterogeneous microstructures when analytical approaches are inappropriate, e.g. due to complicated nonlinear material models, or if local microscopic quantities are searched for in addition to the

effective constitutive response. Also, high phase contrast may indicate the application of numerical homogenization procedures, as many analytical methods can only predict a very broad range of possible behaviours, i.e. the scatter is not practicable. Strategies based on the finite element (FE) method are most common and lead to so-called "FE square" procedures. Fourier-based homogenization schemes are alternatives which are favorable, especially when the representative volume element (RVE) is represented by pixel- or voxel-data, leading to huge data-sets (particularly for the important case of three-dimensional problems).
Originating from the seminal works by Moulinec and Suquet in the 1990s, Fourier-based homogenization has then advanced with respect to two major aspects. Firstly, convergence behavior was significantly improved by replacing the original fixed-point scheme by a standard conjugate gradient (CG) solver pre-conditioned by means of the fast Fourier transform (FFT). Secondly, artifacts evoked by the Gibbs phenomenon were eliminated or reduced by different modifications of the Green's operator, i.e., of the fundamental solution.
A Fourier-accelerated nodal solver (FANS) is presented which makes use of a regular FE mesh and of first-order FE shape functions. FANS can be implemented both as a fixed-point scheme and as a pre-conditioned Krylov method. In contrast to established Fourier-based homogenization schemes, the fundamental solution is given in terms of nodal quantities (e.g., displacements) instead of gradient quantities (e.g., strains). The stiffness matrix is assembled and stored before the iterative procedure is initiated, allowing for savings of computational effort per single iteration. FANS is thus fast but memory-consuming, making it best suited for medium-sized problems. Numerical examples affirm that the solutions converge to FE reference solutions. Hence, the local fields are in particular smooth and devoid of artifacts due to Gibbs' phenomenon. The convergence behavior is studied for varying phase contrasts, including also investigations for heterogeneously distributed Poisson's ratios. Prelimiary results for nonlinear applications including plasticity are presented too. In these cases, benefits of FANS compared to existing methods stand out in particular.

Reduced Basis Homogenization for Hyperelasticity

O. Kunc (EMMA – Efficient Methods for Mechanical Analysis, University of Stuttgart), F. Fritzen (Universität Stuttgart) 15:00

The authors propose an efficient two-scale homogenization method for hyperelastic materials with strong physical nonlinearities (e.g. pseudo-plasticity) in three dimensions. Furthermore, an extension from the geometrically linear to a geometrically nonlinear framework is presented.
A Galerkin-reduced basis (RB) technique is developed in the first part of the presentation. The two main ideas of this approach are

i) the introduction of kinematic fluctuation fields and

ii) a physically motivated and mathematically justified variational formulation of the effective potential.

The approximation of the local fluctuation field (i) by means of a RB allows for the minimization of the effective potential (ii) with respect to these reduced degrees of freedom [1,2]. This procedure results in significant savings in both memory and CPU time. Overall speedups in the order of 10-200 are achieved.

In the second part, we develop a concept for a greedy procedure [3] aiming at reducing the computational complexity of the RB identification. An initially small RB is generated from a set of few pre-calculations performed using FE simulations. The force residuals of the RB model are evaluated along different loading paths. The loadings with the highest estimated error are then subject to supplementing exact computation. The set of pre-calculations is extended by this new data, allowing for the identification of an improved RB.

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Adaptive reduced order models with online error computation

F. Fritzen (EMMA - Efficient Methods for Mechanical Analysis, University of Stuttgart) 15:20

Galerkin reduced order models relying on low-dimensional subspaces of the original solution space can be useful in solving nonlinear mechanical problems: while preserving sufficient accuracy the computation time and the memory demands can both be reduced significantly (see e.g. [1, 2]).
However, the performance of RB methods is limited due to the assembly of the residual vector and (particularly) of the Jacobian. While the effort for the residual vector scales linearly in the reduced dimension N, the effort for the Jacobian is proportional to N^2. Hence, a dimensional reduction within the RB setting can lead to super-linear performance improvements.
This fact is exploited in two stages: First, the RB is locally reduced making the assembly of the residual and the Jacobian computationally less demanding at (next to) no loss in accuracy. Second, nested subspaces of the original RB are considered. The smallest

subspace meeting prescribed accuracy demands is adaptively selected during the online phase. The accuracy is judged on via an a posteriori error measure that is efficiently computed online. Applications for strongly nonlinear hyper-elastic small strain models are presented.

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Recent developments of Fourier-Galerkin Method for Homogenisation of Periodic Media

J. Vondřejc (Technische Universität Braunschweig) 15:40

This contribution is focused on FFT-based method introduced in 1994 by Moulinec and Suquet as an numerical algorithm for homogenisation of periodic media [1]. The method that is originally deduced from Lippmann-Schwinger equation with Green function as an integral kernel has attracted a significant attention because of its computational and memory effectiveness. Recently, the method has been theoretically supported and explained using different discretisation strategies such as Galerkin approximation with piece-wise constant basis functions [2], a collocation method with trigonometric polynomials [3], approximation with finite differences [4], or hexahedral finite elements [5]. Our approach builds on fully variational discretisation [6] using Galerkin approach with trigonometric polynomial basis together with exact numerical integration leading to a scheme with better numerical behaviour than the original scheme [7]. Here we focus on its comparison and similarities to finite element method. The comparison builds upon the energetic norm that exactly corresponds to the error between exact and approximate homogenised material properties. We discuss the influence of the solution regularity on the discretisation and algebraic errors.

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S 8 : Multiscales and homogenization

Tuesday 16:30 - 18:30 Marienstr. 7, 3rd floor, Room 303
Chair: Bernhard Eidel (Universität Siegen)

Computational inelasticity for loading conditions on multiple time scales by adaptive step size control

A. Gote (Universität Siegen), B. Eidel (Universität Siegen) 16:30

Solids and structures may undergo loading histories which exhibit multiple time scales; rather continuous, long-term loading intervals of moderate intensity, which are interrupted by rare, high-intensity, short term loading events. For the numerical analysis of this kind of loading histories, numerical methods must be toughened up to tackle the multiple time scale issue.
Here, we propose an algorithmic solution within a nonlinear finite element framework, which enables the analysis of inelastic solids subject to suchlike particular loading conditions. Time integration of viscoelastic material behavior at finite strains is carried out by a 4th order Runge-Kutta method following the approach in [1] and, in parallel, by the linear Backward-Euler, which on-the-fly provides an estimate of the error in time integration. Adaptive step-size control is directed by the estimated error, which fulfills the requirement of a prescribed, constant accuracy most effectively by time step sizes best adapted to the loading characteristics on disparate time scales.
In representative numerical examples we illustrate the performance of the present method and underpin the computational savings by speed-up factors compared to constant time step sizes.

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consistently couple discretizations in time and space on quadrature-point level for full order p≥2 and a considerable speed-up. Computational Mechanics, 52, 463–483.

Variational sensitivity analysis of physical reaction forces and application to multiscale problems

W. Kijanski (TU Dortmund), F. Barthold (TU Dortmund) 16:50

Sensitivity analysis of mechanical systems plays a key role within applications from structural optimisation. The kind of its theoretical derivation and numerical implementation is responsible for the accuracy and performance of mathematical algorithms for optimisation. Beside *the material derivative approach* (MDA) or *the domain parametrisation approach* (DPA), derivation of necessary sensitivity information using variational principles was proven to be a meaningful method referred to correctness and numerical efficiency. Using formulations proposed in [1], which are fully integrated in the usual representation of continuum mechanics, the effort for the computation of derivatives for quantities of interest is comparable to the effort for the computation of quantities for structural analysis, see [4] for further details. Publications [1, 2, 3] for instance present and discuss essential relations and various beneficial aspects of the variational approach for design sensitivity analysis in detail.
This contribution points out additional remarks and modifications for the derivation of the sensitivity information for physical reaction forces. On one hand the obtained sensitivity information can be used to set up structural optimisation problems on single scales to design support areas of mechanical systems by controlling the amplitude of arising reaction forces. On the other hand this information can be transferred to optimisation problems on multiple scales and can be used to design microstructures. In combination with different well-known and established approaches for analysis and simulation of complex heterogeneous materials on multiple scales based on numerical homogenisation techniques, see [5, 6] and references therein for details, a wide range of applications with design variables, objective functions and constraints on different scales is available and some illustrative examples will be presented.

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A multi-phase/-scale numerical description for industrial, large scale solidification processes

L. Moj (TU Dortmund University), T. Ricken (TU Dortmund University), R. Deike (University of Duisburg-Essen), I. Steinbach (Ruhr-Universität Bochum) 17:10

Numerical simulations of hot working processes, like casting and forming have gained significant importance for steel making industries in order to improve manufacturing. Hence, a continuum-mechanical, bi-phasic, two-scale model has been developed for thermal driven phase transition during solidification processes. The solid and liquid physical states, representing the solid and molten metallic material are formulated in the framework of the theory of porous media (TPM) [1], including thermal coupling [2], finite plasticity superimposed by a secondary power creep law as well as visco-elasticity associated by Darcy's permeability for the solid and the liquid phase, respectively [3]. The phase transition is formulated by a two-scale approach considering the phase-field model on the micro-scale [4]. Here, a double-well potential consisting of two local minima at completely solid and liquid physical states is utilized. The inter-scale, energetic consistent micro-macro linking scheme is formulated, where the Hill-Mandel condition must hold. The finite element method and the finite difference method are employed to solve the macroscopic and the microscopic boundary value problem. The numerical performance as well as its validation is shown by a numerical reproduction of two independent experiments. The first experiment denotes the solidification of a cube-shaped specimen by cooling in air. The second experiment is a controlled cooling of a cylindrical specimen in a Bridgman oven

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Transformation strains for bainitic variant evolution in steel

U. Ehlenbröker[1] ([1]Paderborn University), M. Petersmann[2] ([2]Montanuniversität Leoben), T. Antretter[2] ([2]Montanuniversität Leoben), R. Mahnken[1] ([1]Paderborn University) 17:30

The evolution of the baintic phase in steel is of particular relevance especially in industrial production processes encompassing hot-forming and quenching of larger components. For that reason a multi-scale model for bainitic phase transformation in multi-variant polycrystalline low alloy steels has been developed [1].
In order to yield relasitic simulation results, the microscopic conversion procedures for the austenite-to-bainite transformation have to be described in an appropriate way. To that end, the transformation strains for the crystallographic variants in the model have been adjusted. For the calculation of transformation strains, different theories can be applied, e.g. a hierarchical block-structure as described in [2] for the martenstic phase transformation in a 9Ni-steel, or a theory solely based on the lattice parameters of the two phases (austenite and bainite) and the assumption that the transformation leaves a close packed plane and a close packed direction in that plane unrotated, in other words the measured orientation relationship for the transformation (see [3]).

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A Multiscale Approach with Application to Phase-Field Modeling of Fracture

N. NOII (Institute of Applied Mechanics (CE)), N. NOII (Institute of Applied Mechanics (CE)), L. De Lorenzis (Institute of Applied Mechanics (CE)), O. Allix (Laboratoire de mécanique et technologie), P. Wriggers (Institut für Kontinuumsmechanik) 17:50

The variational approach to fracture by Francfort and Marigo and the related regularized formulation of Bourdin et al. [1], which is also commonly referred to as a phase-field model of fracture, see e.g. the review paper [2], is a widely accepted framework for modeling and computing the fracture failure phenomena in elastic solids. The formulation is non-linear and calls for the resolution of small length scales. Its single-scale treatment is nowadays well-established and shown to be computationally demanding [3, 4]. As such, an idea of multiscale approach that enables to "send" the non-linearity to a lower (local) scale, while dealing with a purely linear problem at an upper (global) one, seems particularly appealing. Clearly, this cannot be realized via

standard homogenization techniques [5] due to a strongly localized phenomenon inherited by the model. In this contribution, we propose a multiscale approach combining the FETI-2LM method [6] and the so-called non-intrusive re-localization formulation [7]. The main novelty here is that we impose the mixed, or, more precisely, the generalized Robin-type boundary conditions [8, 9, 10] to bridge the corresponding scales. In contrast to the Dirichlet boundary conditions being used in [7], this does not lead to a stiff local response, particularly in a softening regime, thus not requiring any "extra efforts" like e.g. relaxation procedures [7]. The important ingredient these mixed conditions (also termed the Dirichlet-to-Neumann map) is an optimal augmented interfaced operator [11], whose construction is, in general, challenging and accomplished in our case using sensitivity analysis. With numerous numerical examples, we show that the proposed two-scale procedure indeed yields results similar to the reference single-scale solution (this includes the entire failure process simulation, as well as the load-displacement curves), yet they are obtained with much superior efficiency. We note that the presented method is (algorithmically) perfectly suitable for the parallel computing concept thus promising further reduction of computational effort.

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Two-Scale Simulation of a Plate with Crack by Using the X-FEM and High-Fidelity Generalized Method of Cells

M. Donhauser (University of Kassel), A. Matzenmiller (University of Kassel), M. Schmerbauch (University of Kassel) 18:10

The two-scale simulation of a plate with a central crack and orthotropic, linear-elastic material behavior is presented under mode-I loading. This simulation serves to verify the X-FEM implementation with orthotropic enrichment functions into the finite element software FEAP. The stress intensity factor is numerically obtained by the interaction integral and compared to the analytical value. Also, the stress at the Gaussian points around the crack tip is compared to the exact solution. The stress and stiffness at each Gaussian point on the macroscale are provided by the high- fidelity generalized method of cells (HFGMC) that is used as homogenization method. So the stress distribution on the finer scale is simultaneously resolved via this micromechanical method called in each integration point. The entire procedure is a first step for the two-scale coupling of the X-FEM and HFGMC before enhancing the approach for a failure analysis of long fiber reinforced composite structures in order to overcome localization effects in simple materials.

S 8 : Multiscales and homogenization

Wednesday 14:00 - 16:00 Marienstr. 7, 3rd floor, Room 303
Chair: Felix Fritzen (Universität Stuttgart)

A two-scale FE-FFT- and phase-field-based model for fully coupled thermo-mechanical problems with heterogeneous and evolving microstructures

J. Kochmann (Institute of Applied Mechanics, RWTH Aachen University), S. Felder (Institute of Applied Mechanics, RWTH Aachen University), S. Wulfinghoff (Institute of Applied Mechanics, RWTH Aachen University), S. Reese (Institute of Applied Mechanics, RWTH Aachen University), B. Svendsen (Microstructure Physics and Alloy Design, Max-Planck Institut für Eisenforschung GmbH) 14:00

Recently, two-scale FE-FFT-based methods [1, 3] have been proposed to predict the local and effective material behavior of heterogeneous materials. The purpose of this work is the extension to fully coupled thermomechanical problems [3] and viscoplastic constitutive modeling. Furthermore, robust Fourier solvers are employed and an efficient solution strategy for two-scale simulations is proposed yielding accurate micromechanical fields and feasible overall CPU times. As an example, the evolution of stress- and temperature-induced martensitic variants in polycrystalline materials is studied for simple macroscopic boundary value problems.

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Homogenization and experimental investigations of pure and fiber reinforced UPPH

L. Kehrer (Karlsruhe Institute of Technology (KIT)), P. Pinter (Karlsruhe Institute of Technology (KIT)), T. Böhlke (Karlsruhe Institute of Technology (KIT)) 14:20

In the sector of lightweight materials, fiber reinforced polymers are applied as resource efficient semi-structural materials. Especially, continuous and discontinuous fiber reinforced thermosets exhibit advantages with respect to their specific material properties, the variety of design freedom as well as the short cycle times regarding the fabrication process. In the work at hand, a composite material based on a thermoset matrix, i.e. polyester-polyurethane hybrid resin (UPPH), reinforced with discontinuous long glass fibers is considered. Fabricated by sheet molding compound (SMC) [1], the microstructure is highly heterogeneous leading, therefore, to an anisotropic material behavior. The thermoviscoelastic material properties are characterized by means of dynamic mechanical analysis (DMA) performed with the GABO Eplexor® 500N for pure and reinforced UPPH specimens. These experiments indicate a temperature-dependent storage modulus but a less pronounced viscoelastic behavior. Thus, the material behavior is thermodynamically modeled with temperature-dependent elasticities. The effective thermoelastic material properties of this discontinuous long fiber reinforced composite are approximated using the homogenization scheme by Mori and Tanaka [2, 3], formulated explicitly in terms of orientation averages. This allows to use orienation tensors of 2nd and 4th order describing the orientation information on the micro level. The orientation tensors are obtained by computed tomography scans [4]. Finally, a comparison and a discussion is given for the experimental results by DMA for several temperature loads and the homogenized simulation results by applying the Mori-Tanaka method.

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Efficient Simulation of Short Fibre Reinforced Composites

R. Springer (TU Chemnitz), A. Meyer (TU Chemnitz) 14:40

Lightweight structures became more and more important over the last years. One special class of such structures are short fibre reinforced composites, produced by injection moulding. To avoid expensive experiments for testing the mechanical behaviour of these composites proper material models are needed. Thereby, the stochastic nature of the fibre orientation is the main problem.
In this talk we look onto the simulation of such materials in a linear thermoelastic setting. So, we use the stress-strain relation

$$\sigma = \mathfrak{C} : (\varepsilon - (\theta - \theta_0)\mathbf{T}),$$

with a fourth order material tensor $\mathfrak{C}$, a second order thermal expansion tensor $\mathbf{T}$, the temperature difference $(\theta - \theta_0)$, and the second order linearised strain tensor ε.
The needed material properties can be described by averaging the material properties of transversely isotropic materials. In this talk we will present how this can be used for the description of the arising stresses within such composites.
Furthermore, we look onto the above equation in a time dependent setting, i.e. θ is described by

$$c_\rho \rho \frac{\partial \theta}{\partial t} - \nabla(\cdot\kappa \cdot \nabla\theta) = \Theta,$$

with the material density ρ, the specific heat capacity c_ρ and the symmetric second order heat conduction tensor κ. Here, κ also depends on the stochastic fibre orientation.

Comparison of mean field homogenization schemes for short fiber reinforced thermoplastics

P. Hessman (Robert Bosch GmbH), K. Hornberger (Robert Bosch GmbH) 15:00

Models for the simulation of short fiber reinforced thermoplastic (SFRT) composites need to account for the heterogeneity and complex microstructural morphology of these materials. This is often done by means of computational homogenization schemes which rely on representative volume elements and typically large finite element models to solve for micromechanical fields, such as stresses and strains, and effective macroscopic properties. While highly accurate with respect to the microstructural setup, these models are most often not viable for the simulation of real parts. On the other hand, mean field homogenization schemes are less computationally expensive, while still accounting for the microstructural composition in an averaged manner and being capable of yielding information about inclusion stresses and strains.

This work focuses on applying different mean field homogenization schemes to SFRT composite materials. We consider polybutylene terephthalate reinforced with short glass fibers and a fiber mass fraction of 30%. Experimental results from tensile tests are used, which were performed on specimens cut out of injection-molded plates at different angles from the main mold flow direction. The microscopic state within the material was resolved by means of x-ray micro-computed tomography (μCT) and enters the models via fiber orientation distributions and fiber length information. We evaluate the stiffness tensors predicted by the different mean field homogenization schemes and compare them to the direction-dependent experimental moduli. The influence of the different microstructural parameters (e.g. the layer-wise fiber orientation tensors) is assessed with regard to the effective elastic properties and inclusion stresses and strains.

An efficient multiscale method for computing the effective viscoelastic response of short fiber reinforced thermoplastics

J. Köbler, M. Schneider, H. Andrä (Fraunhofer Institut für Techno- und Wirtschaftsmathematik) 15:20

Short fiber reinforced plastics constitute an important and widely used class of materials, due to their stiffness and strength properties as well as their low specific weight. The elastic and inelastic material properties of injection molded parts depend strongly on the local fiber orientation which is continuously varying.
Multiscale simulations provide insight into the creep and relaxation behavior of these components. Due to the high length-diameter ratio of fibers, resolving individual fibers is prohibitive. We present a two-step approach, based on the generation of effective models for sample fiber orientations, which are subsequently interpolated to ensure the calculation of the effective mechanical properties for a general fiber orientation.
To demonstrate the efficiency of this scheme we investigate linear viscoelasticity described by Burgers' model focusing on the creep and relaxation behavior of short glass fiber reinforced polyamide 66. The anisotropic linear viscoelastic ersatz models for a single fiber orientation are generated using Schapery's Collocation method in conjunction with an FFT-based homogenization scheme.

The effective shear modulus for an n-layered composite sphere

P. Lenz (Universität Paderborn), R. Mahnken (Paderborn University), C. Dammann (Paderborn University) 15:40

This work presents the derivation of the effective shear modulus for a heterogeneous material composed of multi layered composite spheres embedded in a linear elastic matrix. The derivation is based on the *composite spheres model* known from the literature [2]. The heterogeneous material is subjected to both, a *shear stress* in a stress approach and a *shear deformation* in a displacement approach, respectively. In contrast to [1], [2] and [3] the effective shear modulus is obtained by equating the results of two models as in [4]. In the first model, the heterogeneous sphere is embedded in an *equivalent homogeneous* material; in the second model, the heterogeneous sphere is replaced by an equivalent homogeneous sphere. Then the stresses or respectively the strains of the

homogeneous and the heterogeneous sphere resulting from the related boundary value problems, are equated for the stress and the displacement approach. For each approach this results into an over-determined system of equations which to solve with the least square method.
In a numerical study for a (2) and (3)-layered composite spheres it is demonstrated that both solutions lie within the Voigt and Reuss bounds, respectively. It is also shown that the shear stress approach coincides with the solution given by [1] as well as the extension to the n-layered composite sphere model given by [3]. Furthermore, we show that the semi analytical-numerical solution for the shear displacement approach yields an upper bound, whereas the shear stress approach yields a lower bound.

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S 8 : Multiscales and homogenization

Wednesday 16:30 - 18:30 Marienstr. 7, 3rd floor, Room 303
Chair: Bernhard Eidel (Universität Siegen)

Derivation of (n)- and (n+1)-layered composite sphere models for thermo-chemo-mechanical effective properties

C. Dammann (Paderborn University), R. Mahnken (Paderborn University), P. Lenz (Universität Paderborn) 16:30

Our work presents extensions of multi layered *composite sphere models* known from the literature [1, 2, 3] to temperature-dependent elastic effects accompanied by curing. Volumetric effective properties in dependence on the degree of cure are obtained by homogenization for a representative unit cell (micro-RVE) on the heterogeneous microscale. To this end, analytical solutions for (n)- and $(n+1)$-layered composite sphere models, [3, 4], are derived, in addition to Voigt and Reuss bounds resulting from the assumption of a homogeneous mixture. For simplification, we restrict the material behavior of the

micro-RVE to thermo-chemo-mechanical coupling with linear elasticity. As a further result the equivalence for the thermo-chemo-mechanical volumetric effective properties of the (n)- and $(n+1)$-layered composite sphere model is shown. Moreover, in a numerical study it is demonstrated that the effective elastic and thermal properties lie within bounds, whilst for the chemical part of the model, an analogous result is obtained for the effective strains.

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Multiscale modeling of fiber reinforced composites under compressive loading

T. Hanisch (Technische Universität Darmstadt, Fachgebiet Festkörpermechanik), F. Gruttmann 16:50

A mechanism of fiber failure under axial compression in an unidirectional layer is fiber buckling on the microscale. Assuming that the system is perfect this failure is a stability problem. For such kind of problems it is not sufficient to model an unidirectional layer with transversally isotropic material data.
Thus in this work a coupled two-scale model for fiber reinforced composites is presented. On the macroscale a fiber reinforced composite is modeled geometrically linear under axial compression, whereas on the microscale a representative volume element (RVE), existing on a fiber embedded in a matrix material is modeled geometrically nonlinear. The discretization on both scales is performed with brick elements and on the RVE periodic boundary conditions are applied. A variational formulation and their linearization of the FE^2 problem is derived. On the microscale the influence of length of the RVE and the influence of an imperfection on the microscale are discussed. The numerical results are compared with experimental data.

An adaptive approach for modeling a fiber-matrix composite with the FE² method

M. Praster (RWTH Aachen University), S. Klinkel (RWTH Aachen University) 17:10

The contribution deals with an adaptive concept for the Finite-Element-Square (FE^2) method. Therefore, a fiber-matrix composite material is considered. This material

has typically a complicated random fiber distributed microstructure, with unknown macroscopic material properties. In the present contribution elasto-plastic material behavior is considered for the fibers. Thus, the stress response depends nonlinear on the deformation and the fiber orientation. A homogenization of the fiber-matrix composite on the microscale leads to the macroscopic material properties. The nonlinear material behavior of the fibers necessitates an accompanying homogenization process. In the present work, this is realized in the frame of a FE^2 formulation. It combines two nested finite element simulations. On the macroscale, the boundary value problem is modelled by finite elements, at each integration point a second finite element simulation on the microscale is employed to calculate the stress response and the material tangent modulus. One huge disadvantage of the approach is the high computational effort. Certainly, an accompanying homogenization is not necessary if the material behaves linear elastic. This motivates the present approach to deal with an adaptive scheme. An indicator, which makes use of the different boundary conditions (BC) of the BVP on microscale, is suggested. The homogenization with the Dirichlet BC overestimates the material tangent modulus whereas the Neumann BC underestimates the modulus. The idea for an adaptive modeling is to use both of the BCs during the loading process of the macrostructure. Starting initially with the Neumann BC leads to an overestimation of the displacement response and thus the strain state of the boundary value problem on the macroscale. An accompanying homogenization is performed after the strain reaches a limit strain. Dirichlet BCs are employed for the accompanying homogenization. Some numerical examples demonstrate the capability of the presented method.

Error-controlled homogenization for a class of linear elastic composite problems

X. Ju (University of Paderborn), R. Mahnken (University of Paderborn) 17:30

The notion of model adaptivity has been well established, aiming at adaptive selection of mathematical models from a well defined class of models (model hierarchy) to achieve a preset level of accuracy (see e.g. [1,2]). The present contribution addresses its application to a class of linear elastic composite problems. We will show that the classical bounding theories according to [3,4] can provide a model hierarchy in a natural and theoretically consistent manner, without combination of different methods using a priori knowledge. As a further benefit, the resulting computational scheme reduces to a single-scale one. To arrive at computable higher order bounds, the classical singular approximation following [5] is made. As a new finding, this may, under certain circumstances, give rise to an overlap effect. To overcome this, a correction is proposed. Additionally, the model adaptivity is coupled to the well established adaptive finite element method (FEM), such that both macro model and macro discretization errors are controlled. The proposed adaptive procedure is driven by a goal-oriented a posteriori error estimator based on duality techniques. For efficient computation of the dual solution, a patch-based recovery technique is proposed. For illustration, numerical examples are presented.

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adaptive modeling of heterogeneous materials: I. Error estimates and adaptive algorithms, *Journal of Computational Physics*, 164(1), 22–47 (2000).

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Modelling the thermal conductivity of CNT composites

M. Nagaraj (Ruhr Universität Bochum), J. Timothy (Ruhr Universität Bochum), G. Meschke (Ruhr Universität Bochum) 17:50

The thermal conductivity of a carbon nanotube composite material is strongly influenced by the volume-fraction, distribution and shape of the dispersed CNT (carbon nanotube) inclusions. For an REV with an isotropic distribution of idealized, straight CNT inclusions with a certain aspect-ratio, the effective thermal conductivity is estimated using the cascade scheme at the self-consistent/self-similar limit [2, 3] taking into account the influence of defects at the scale of a single CNT using lattice micromechanics [1]. To take into account the effect of CNT crumpling, an effective CNT aspect-ratio is computed as a function of CNT crumpling using computational homogenization of a numerical REV using the Voxel-FE method. The numerical REV's are generated using an image based algorithm by specifying the degree of crumpling (crumple factor) and the length, thickness of the CNT's. The model predictions are validated using available experimental data.

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[3] Timothy, J. J. & Meschke, G. (2016): A cascade continuum micromechanics model for the effective elastic properties of porous materials. International Journal of Solids and Structures 83, 1-12

Homogenization of metamaterials: Application and limits of a new generalized homogenization scheme

C. Findeisen (Karlsruher Institut für Technologie), J. Hohe (Fraunhofer Institut für Werkstoffmechanik), P. Gumbsch (Karlsruher Institut für Technologie) 18:10

Metamaterials are characterized by effective properties which are mainly driven by the topology of the microscopic structure and less by the properties of its constituents. Many unusual and interesting effective material properties can be realized, by for example exploiting structural instabilities [1]. However, until today metamaterials are mostly analysed by the microstructure only, and a systematic material description is lacking.
Aiming at a continuum description of mechanical metamaterials, we derive a general homogenization scheme for higher order continua. Coupling between micro and macro strain energy is given by an extension of the Hill-Mandel condition [2] and a link between micro deformation and effective strain measures is introduced by the solution of a minimization problem [3]. However, in contrast to existing approaches, the latter condition is fulfilled without any further assumptions on the microfluctuation field. This is especially important in the case of metamaterials, where an overconstrained microstructure can have a significant influence on the effective behaviour. Both, applicability and limits of the presented approach are demonstrated with some analytical and numerical examples.

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S 8 : Multiscales and homogenization

Thursday 14:00 - 16:00 Marienstr. 7, 3rd floor, Room 303
Chair: Stefan Löhnert (Leibniz Universität Hannover)

From particle mechanics to microcontinuum theories

S. Bidier (University of Stuttgart), W. Ehlers (University of Stuttgart) 14:00

Microcontinuum theories enable the consideration of particle-based microstructures within a continuum mechanical framework. Several classes of microcontinua, such as the micromorphic, the micropolar, the microstrain or the microstrech formulation, have been successfully applied to engineering applications, although a clear physical determination and

interpretation of the kinematical extensions and the resulting higher-order stresses within the formulation is frequently missing. In this regard, the present contribution focuses on establishing the physical link between discrete contact forces, stresses and deformation of particle-based microstructures and the characteristic stress states of microcontinuum theories. Representative Elementary Volumes (REVs) are therefore constructed on the mesoscale as ensembles of deformable particles from the mircoscale. Establishing the REV balance relations justifies the common generalisation of the angular momentum balance commonly applied in microcontinuum theories, leads to the identification of the continuum stresses based on micro-quantities and furthermore enables the application of homogenisation techniques by exploitation of the equilibrium conditions of a REV.

In order to investigate the hereby established link from the micro- to the macroscale, granular materials are simulated using the Discrete-Element Method (DEM). In particular, localisation phenomena in granulates, e. g. in biaxial compression tests or during ground-failure processes are studied. This implies the formulation of the contact between particles in an appropriate constitutive manner in accordance to the envisaged granular material behaviour, e. g. whether loose material, such as sand, or bonded multi-component material, such as polyurethan-sand compounds for metal casting applications are of interest. With the full solution of a particle-based initial-boundary-value problem, the homogenisation formalism is applied and enables the study of the extended continuum field quantities, essentially demonstrating the applicability of microcontinuum theories in the field of granular material.

Micromorphic homogenisation and its application to a model of ductile damage

G. Hütter (TU Bergakademie Freiberg) 14:20

Ductile failure of metals is a consequence of nucleation, growth and coalescence of voids. Due to its relevance in engineering applications, a large number of constitutive models were developed to describe this mechanism. Among them, the models of Gurson and Rousselier and its numerous modifications are the most prominent ones. However, both models are formulated within the theory of simple materials and thus do not contain an intrinsic length. That is why the problem becomes ill-posed in the softening regime manifested in a spurious mesh dependency in corresponding FEM simulations. Nonlocal and gradient-enriched extensions of these damage models were proposed to overcome this problem. However, most of these extensions are purely heuristical and the additional terms and constitutive parameters lack a distinct micromechanical basis. In contrast, the model of GLPD model [1] was derived analytically from homogenization within the theory of strain-gradient media so that the mean distance of voids as intrinsic length enters naturally. However, the FEM implementation of strain-gradient theories raises certain difficulties and is expensive.
Both, implcitely gradient-enriched nonlocal theories and strain-gradient theories are special cases of the micromorphic theory. It would be desirable to combine the advantages of both approaches, i. e. to have a model of ductile damage which combines a

sound micromechanical basis, including the intrinsic length, with an efficient numerical implementation. For this purpose, the theory of micromorphic homogenization [2] is confined to microdilatational media. An adaption of Gurson's limit load analysis of an RVE with void to the microdilatational framework yields a extended damage model of Gurson-type whose yield condition contains the intrinsic length and non-classical stress measures naturally. The model is implemented into a multi-purpose FEM code.

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Modeling wave propagation in real phononic crystals via the relaxed micromorphic model

A. Madeo (INSA-Lyon), P. Neff (University of Duisburg-Essen) 14:40

We discuss the interest of using enriched continuum models of the micromorphic type for the description of dispersive phenomena in metamaterials. Dispersion is defined as that phenomenon according to which the speed of propagation of elastic waves is not a constant, but depends on the wavelength of the traveling wave. In practice, all materials exhibit dispersion if one considers waves with sufficiently small wavelengths, since all materials have a discrete structure when going down at a suitably small scale. Given the discrete substructure of matter, it is easy to understand that the material properties vary when varying the scale at which the material itself is observed. It is hence not astonishing that the speed of propagation of waves changes as well when considering waves with smaller wavelengths. In an effort directed towards the modeling of dispersion in materials with architectured microstructures (metamaterials), different linear-elastic, isotropic, micromorphic models are introduced and their peculiar dispersive behaviors are discussed by means of the analysis of the associated dispersion curves. The role of different micro-inertias related to both independent and constrained motions of the microstructure is also analyzed. A special focus is given to those metamaterials which have the unusual characteristic of being able to stop the propagation of mechanical waves and which are usually called band-gap metamaterials. We show that, in the considered linear-elastic, isotropic case, the relaxed micromorphic model, recently introduced by the authors, is the only enriched model simultaneously allowing for the description of non-localities and multiple band-gaps in mechanical metamaterials. We finally propose to apply our relaxed micromorphic model to the study of real phononic crystals thus showing how the proposed model is able to effectively describe band-gaps in realistic scenarios. This comparison with experimental results allows for the fitting of the parameters of the considered model for specific band-gap metamaterials by inverse approach. This fitting, when successfully concluded for some specific metamaterials will allow the setting up of the design of metastructures (i.e. structures which are themselves made of

metamaterials) by means of tools which are familiar to engineers, such as Finite Element codes.

Investigation of discrete stress distribution for dry powder compaction using discrete element modeling, weighted Voronoi tesselation and homogenization

S. Rasche (MFPA Weimar), C. Könke (MFPA Weimar), A. Tahir (MFPA Weimar) 15:00

Powder compaction of granular material plays a substantial role in the manufacturing processes of ceramics industry and powder metallurgy industry. Pourable granular powder (ceramic powder of metallic powder) is filled into a die or mould and compacted through the application of high pressures. The mechanical properties of the compacted green part is ruled by its granular microstructure, which is a result of polydisperse granular material behaviour and applied boundary conditions. Discrete element method (DEM) allows one to investigate the powder compaction process numerically on the microscale by modeling the forces on the particle level and simulating the particle motion. Three-dimensional data about particle size distribution and spatial structure of the particle packing can be extracted from micro-computed tomography (µCT). The connection of the discrete micro-description and the macro-description using continuum theories is a challenging task. An average stress tensor can be computed from DEM results, evaluating the contact forces and the distances from the particle center to the contact point with respect to an average cell volume [1, 2]. Instead of using a grid of cells for homogenization, we apply a weighted-voronoi tesselation technique for defining the cell volume with respect to each individual particle. Local bulk density as well as local void fraction can be computed by the way. With this approach all structural information (size, position and neighbors of individual particles, particle interaction forces) can be transferred to a continuum description of heterogeneous microstructure, suited for multiscale finite element modeling. Computed discrete stress fields at different stages of powder compaction process will be presented together with data about corresponding particle size distribution and spatial structure of particle packings.

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A two-scale homogenisation approach for fluid saturated porous media based on TPM and FE²-Method

F. Bartel, T. Ricken (TU Dortmund University), J. Schröder (Duisburg-Essen University), J. Bluhm (Duisburg-Essen University) 15:20

Thinking about the description of porous materials, e.g. metal foam, human tissue, plants or sponges, we always have to take into account a global design composed of various substructures with different characteristics on a lower level. Examples of such substructures are pores which can be saturated with fluids or gases, fibres with different orientations or cells which can be influenced by chemical reactions. For the theoretical

description of the behaviour, enhanced continuum mechanical models give promising approaches. Up to now, due to the high complexity, it has not been possible to simulate these systems with only one design model. Hence, it is necessary to think about techniques which simplify the model but still consider the essential characteristics.
It is clear, future applications will consider the discrete microstructure of materials. For example the topology can be received by CT-scanning and therefrom Representative Volume Elements (RVEs) can be designed. Therefore, we are preparing the Theory of Porous Media (TPM) for the usage in combination with the FE^2-Method.
This contribution will present a two-scale homogenisation approach for fluid saturated porous media with a reduced two-phase material model, which covers the behaviour of large poro-elastic deformation. The main aspects of theoretical derivation for the weak form, the lower level boundary conditions under consideration of Hill-Mandel homogeneity condition and the averaged macroscopic tangent moduli will be pointed out and a numerical example will be shown.
Still, solving a coupled problem in FE^2 environment is extremely time consuming, therefore a parallel solution strategy is absolutely essential and remarks on the investigation of High Performance Computation in this context will be given.
Finally, creating a suitable geometric model and finite element mesh, for the macroscopic as well as for the microscopic structure, of a real problem will be mandatory. Hence, we present the mentioned procedure of transferring CT .raw images to a FE-model on an example of a concrete specimen.

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Coarse Grid CFD: a homogenization technique to tackle indutrial scale problems

F. Yu (Karlsruhe Institute of Technology (KIT)), A. Class (Karlsruhe Institute of Technology (KIT)), J. Xiao (Karlsruhe Institute of Technology (KIT)), T. Jordan (Karlsruhe Institute of Technology (KIT)) 15:40

For a given flow related problem, we assume $\mathbb{L}_1\mathbf{u}_1 = \mathbb{N}_1(\mathbf{u}_1)$ defined on fine mesh, while $\mathbb{L}_2\mathbf{u}_2 = \mathbb{N}_2(\mathbf{u}_2)$ defined on coarse mesh. Between the two results of the numerical simulation, an inviscid Euler Equation based Coarse-Grid CFD(CGCFD) method is set up, which ensures $< \mathbf{u}_1 >_m = < \mathbf{u}_2 >_m$, where $<>_m$ denotes the average evaluated on mesh cell m of the coarse mesh. During the process, a homogenized sub model, derived from detailed Navier-Stokes level simulation, is automatically constructed, together with Coarse-Grid solver (i.e. $\mathbb{L}_2$, $\mathbb{N}_2$), to filter sub-grid scales, while maintaining the consistence and accuracy of results for the anticipated industrial level application. For validation, we apply the developed methodology to a simple test case and an industrial scale application, e.g. a 127 pin wire-wrapped rod bundle.

S 8 : Multiscales and homogenization

Thursday 16:30 - 18:30 Marienstr. 7, 3rd floor, Room 303
Chair: Stefan Löhnert (Leibniz Universität Hannover)

Micro-to-macro transition accounting for general imperfect interfaces

A. Javili 16:30

The objective of this presentation is to establish a micro-to-macro transition framework to study the behavior of heterogeneous materials whereby the influence of the interface at the micro-scale is taken into account. The term “interface” refers to a zero-thickness model that represents the finite thickness “interphase” between the constituents at the micro-scale. Therefore, the interface is essentially a two-dimensional manifold embedded in a three-dimensional Euclidean space. Due to increasing area-to-volume ratio with decreasing size, the interface assumes a more pronounced effect on the material response at small scales. Hence, it is of crucial importance to account for interfaces at the micro-scale. We show that including the interfaces at the micro-scale introduces a length-scale into the first-order computational homogenization. Our interface-enhanced computational homogenization framework captures the size effect in the material response that is missing in the classical computational homogenization.
The interface model in this contribution is general imperfect. Within the continuum mechanics setting, interface behavior is often described using the *cohesive zone model* or *interface elasticity theory*. The cohesive zone model allows for the jump in the deformation field across the interface but, restricts the traction jump to vanish. On the contrary, the interface elasticity theory permits the traction jump across the interface, however, it is only valid for coherent interfaces and thus, no displacement jump at the interface is allowed. We propose a general imperfect interface model and show that both cohesive zone model and interface elasticity theory can be derived as two limit cases of this general model.
Furthermore, computational aspects of general imperfect interfaces using the finite element method are detailed. We establish a consistent computational homogenization

scheme accounting for general imperfect interfaces. Suitable boundary conditions to guarantee meaningful averages and bridging between the scales are derived. Clearly, our general framework reduces to classical computational homogenization in its most elementary limit. Finally, the proposed theory is elucidated via a series of numerical examples.

Continuum modeling of material interfaces and material surfaces based on an atomistic description

C. Sievers (TU Dortmund), J. Mosler (TU Dortmund) 16:50

In many applications, material interfaces and material surfaces significantly influence the effective mechanical properties of the considered material. Ultra fine grained steels are representative examples. Unfortunately, the mechanical properties of material interfaces and surfaces are difficult to be measured. Alternatively, they can be predicted with high accuracy by means of atomistic simulations. However, due to the underlying numerical complexity, atomistic simulations are often not possible at the relevant macroscopic scale. In this talk, a multiscale approach is elaborated linking the atomistic to the macroscopic scale. It relies on the principle of energy equivalence, combined with a Ritz-type approximation.

Contact Mechanics in Computional Homogenization

A. Leichner (Fraunhofer Institut für Techno- und Wirtschaftsmathematik), H. Andrä (Fraunhofer Institut für Techno- und Wirtschaftsmathematik), B. Simeon (Technische Universität Kaiserslautern) 17:10

The purpose of numerical homogenization of composite materials is to compute effective macroscopic material parameters [1], while micromechanical problems are considered in so called representative volume elements (RVE). In an RVE microstructures are often obtained from digital images, such that deformable objects are embedded into a mesh built of voxels. As a result, this representation in a Cartesian grid does not demand any expensive meshing technique and need not to consider common problems known for standard finite elements. Besides, a discretization into uniform voxels allows to apply the fast Fourier transform (FFT) in order to precondition the arising linear system of equations and finally to solve both linear and nonlinear mechanical problems fast and efficiently.

Nonlinear stress responses, like contact stresses, often falsify the computed effective properties from homogenized results, if not treated correctly. Consequently, homogenization methods have to consider (possibly a lot of) collisions between solid materials, too, when dealing with porous media. But the discretization into voxels complicates computations on surfaces and interfaces, which become even more cumbersome, when large deformations have to be considered. In this case the contact surface might change per load step and has to be defined a priori.

In the past decades the numerical treatment of contact problems has been intensively

investigated for the finite element method using an unstructured grid. On the contrary, a thorough research for voxel based methods is still at its beginnings. So recent results have been published in context with arbitrary Lagrangian-Eulerian (ALE) methods [2]. Solutions are presented there which use mixture theories or coupled multi-material displacement fields. Nonetheless, these approaches either do not give satisfying results (mixture ansatz) or are not applicable to FFT-based methods (coupled solution fields). Additionally, a proper collision detection in terms of distances is still missing and contact is not considered as a reaction force between two surfaces.
Therefore, we present in this contribution ideas which are basically known for finite element methods and are still compatible with a fast, voxel based elasticity solver. Before we turn to the actual solution of contact problems, we will introduce an Eulerian formulation of distances between objects, which are obviously the most important criteria for contact detection. This formulation is better known as level set representation or signed distance function [3]. The well known Fast Marching Method and Level Set Method are suitable tools to compute a distance function or to advance it in time by the displacements. Moreover, a distance function enables an efficient detection of contact zones, where the necessary contact conditions are treated.
With the aid of level set data, we demonstrate how these conditions can be fulfilled by standard solution techniques, like the penalty method, such that contact problems can be solved on this kind of discretization. Furthermore, we show how to improve the accuracy by a Nitsche based ansatz and how problems with large deformations can be treated with an ALE approach. In the end, the solutions of a benchmark problem will be discussed and analyzed in order to demonstrate the efficiency of the proposed methods.

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[2] E. Vitali, D. J. Benson: An extended finite element formulation for contact in multi-material arbitrary Lagrangian-Eulerian calculations, *Int. Journ. Num. Meth. Engng*, 67, 1420-1444 (2006)

[3] J.A. Sethian: Theory, Algorithms and Applications of Level Set Methods for Propagating Interfaces, *Acta Numerica* (1995)

Multiscale Rubber Friction Analysis on Rough and Flexible Surfaces

F. Hartung (Technische Universität Dresden), M. Kaliske (Technische Universität Dresden) 17:30

Friction is a complex phenomenon and has a significant importance in daily life. One main field of research is associated with tire industry, because tire-pavement interaction affects every driving maneuver. Hence, it is important to understand the physical background on different length scales. Friction in general consists of different contributions - hysteresis friction, adhesion, viscous friction and interlocking effects. One significant part

of friction is the so-called hysteresis effect as a consequence out of the internal dissipation of the viscoelastic material which also depends on slip velocity, contact pressure and temperature.

Due to the different asperities of a rough surface, e.g. asphalt pavement, it is necessary to consider the entire frequency spectrum or length scales. With both, the height difference correlation function (HDCF) and the power spectral density function (PSDF), it is possible to characterize a rough surface texture [1]. With a certain number of sinusoidal functions, the surface can be approximated out of the HDCF or the PSDF. A multiscale approach can provide friction features on each length scale to accumulate the micro- and mesoscopic friction into a macroscopic friction coefficient [2]. By using the finite element method (FEM), the sensitivity of the influencing factors, for instance slip velocity and contact pressure, may be investigated for the two- and the three-dimensional case.

Different approaches exist to consider the constitutive behavior of both contact partners, e.g. the tread material and the pavement structure below. In general, a finite linear viscoelastic model based on Prony-series is used to model rubber materials [3]. The pavement surface is often assumed as a rigid body in which no dissipation effects out of the road are taken into account. A comparison between a rigid and a flexible pavement model provides information about the impact of the road deformation on the resulting hysteresis friction features.

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Numerical study of adhesive and cohesive failure of structured interfaces

F. Hirsch (Technische Universität Dresden), M. Kästner (TU Dresden) 17:50

Multi-material lightweight designs, e.g. the combination of aluminium with fibre-reinforced composites, are a key feature for the development of innovative and resource-efficient products [1]. Among established technologies like bolt joints, interlocking non-destructive approaches are promising solutions. The connection properties of such bi-material interfaces are influenced by the geometric structure on different length scales.
In this contribution, a numerical study is presented, which addresses the failure behaviour of structured interfaces within a computational homogenisation scheme [2]. Different local phenomena, e.g. the surface roughness and different local failure types like

cohesive failure of the polymer and adhesive failure of the local interface and their effects on the overall interface characteristics are investigated. The roughness is idealised by simple profile geometries to relate the resulting macroscopic adhesion to the individual parameters on the microscale. Adhesive interface failure is modelled by cohesive elements based on a traction-separation law and cohesive failure of the bulk material is described by an elastic-plastic model with progressive damage evolution.
Since there is a large separation in the length scales of the surface roughness, which is in the micrometre range, and conventional structural components, we employ a numerical homogenisation approach [3] to extract traction-separation laws in macroscopic normal and tangential direction to derive effective interface parameters.

Acknowledgements:
The present project is supported by the German Research Foundation (DFG) within the Priority Programme (SPP) 1712. This support is gratefully acknowledged.

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Multiscale Approach for Modelling Heat Affected Zones of Welded Joints

I. Wudtke (Bauhaus-Universität Weimar), M. Silani (Isfahan University of Technology), M. Kraus (Bauhaus-Universität Weimar) 18:10

Two-dimensional hierarchical multi-scale approach will be presented for modelling heat affected zones (HAZs) of welded connections. Therefore metallurgical constituents have been identified and validated using experimental analyses, i.e. micro-sections, measured Vickers-hardness profiles and Time-Temperature-Transformation diagrams of the parent material. The identified constituents have been used in the hierarchical two-scale approach (meso-macro-scale) for the calculation of effective stress-strain relations in particular spots of the HAZ and parent material. Images of real micro-structure for investigated points of the HAZ have been used for the generation of representative volume elements (RVEs). Numerical calculations based on these RVEs have been performed taking a plane strain state and isotropic material behavior into consideration as well as linear displacement boundary conditions. Since the microscopic constitution of a HAZ is changing gradually with the increasing distance from the weld, the calculated stress-strain curves are representing the effective material behavior in discrete points of

HAZs. For the numerical representation of this phenomenon, which is defined as a special case of morphologic texture here, a spatial grain size function (GSF) has been identified, using regression analysis methods. The material properties of HAZs on macroscopic scale change discretely at every material point with respect to the GSF. As a practical example, the spatial distribution of effective material properties has been evaluated and the modelling strategy has been applied on the HAZ of butt welded joints of two-phase fine grained steel S460. A numerical simulation of a tensile test performed on these welded joints has been undertaken and the obtained results are discussed and compared to experimental data.

S 9: Laminar flows and transition

Organizers: Gunther Brenner (TU Clausthal)
Bettina Frohnapfel

S 9 : Laminar flows and transition

Tuesday 14:00 - 16:00 Marienstr. 13, 1st floor, Lecture hall D

The influence of a DC electric field on the von Kármán vortex street in the wake of a confined cylinder

M. Scholz (Queen's University at Kingston), S. Hardt (TU Darmstadt), D. Barz (Queen's University at Kingston) 14:00

The von Kármán vortex street is a flow instability that is observed in the wake of a blunt body if a certain Reynolds number is exceeded. It is one of the classical fluid mechanics problems and a vast amount of research has been dedicated to the investigation of the fundamentals of this phenomenon. The present study is concerned with the numerical simulation of the pressure-driven flow around a confined cylinder subjected to a DC electric field. In this setup, two distinctions to the classical von Kármán vortex street can be noted. On the one hand, the confinement of the flow field differs from its unbounded counterpart because of the shear in the incoming velocity profile, shear induced in the vicinity of the boundaries, and with the impermeability of the vortices through the channel walls. On the other hand, the electric field induces a small but finite electrokinetic velocity very close to the cylinder surface contrary to the flow situation arising from the no-slip velocity in the conventional case. Various numerical simulations are performed in the Laminar Vortex Shedding Regime to investigate the influence of the Reynolds number, cylinder-diameter-to-channel-width blockage ratio and the direction of the electric field. In case of no electric field, the blockage ratio shifts the critical Reynolds number to higher values. Likewise, the dimensionless shedding frequency (Strouhal number) at a given Reynolds number increases with increasing blockage ratio. In case of an applied constant electric field, the simulations reveal that the time to reach a

steady Laminar Vortex Shedding Regime is reduced compared to a pure pressure-driven flow with the identical Reynolds number while the dimensionless shedding frequency remains the same. The reason for the reduction of the transient is related to the different flow topologies around the cylinder. The electrokinetic velocity disturbs the axial flow symmetry of the Laminar Steady Regime and therefore accelerates the onset of the Laminar Vortex Shedding Regime.

Large Eddy Simulation with Stabilized FEM for Transition and Turbulence in Medical Devices

L. Pauli (RWTH Aachen University), M. Behr (RWTH Aachen University) 14:20

Common medical devices like blood pumps operate in flow regimes, where laminar and turbulent flows occur at the same time. Especially, the transition regions between laminar and turbulent flow are very difficult to capture numerically. As RANS-based models are known to behave poorly in such flow regimes, we focus on state-of-the-art LES modeling to capture the complex flow patterns. In particular, two LES turbulence models are considered: the σ-model and the variational multiscale turbulence model.
The σ-model is an eddy-viscosity based, subgrid-scale model. Its definition is based on the singular values of the resolved velocity gradient and particularly simple. By construction, the eddy-viscosity vanishes if the resolved flow field is two-dimensional or two-component and is shown to have the proper near-wall behavior. The σ-model is shown to perform similar (or even better) than the Dynamic Smagorinsky model [1].
The variational multiscale turbulence model is an extension of the stabilized finite element concept. The flow solution is decomposed into resolvable (coarse) and unresolvable (fine) scales by the FE approximation. While the coarse scales are computed by standard FE approaches, the fine scales are approximated by normalized residuals of momentum and mass. This way, new stabilization terms are added to the variational formulation that can be interpreted as cross and Reynolds stresses known in turbulence theory [2].
The turbulence models are tested in a simple nozzle benchmark device, where PIV data is available. The nozzle, consisting of a conical convergent, a throat, and a sudden expansion, mimics flow fields in several medical devices, such as flow contraction and expansion, flow recirculation, and regions with laminar and turbulent flow. The comparison is performed for a Reynolds number of 3500.
We will also present a full blood pump simulation with available experimental data. In such computations, additional methods like the multiple-reference-frames (MRF) [3] method or ALE-based mesh motion are considered.

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Simulation of solidification processes in viscoelastic polymer melt flows

S. Descher (University of Kassel), O. Wünsch (University of Kassel) 14:40

In this contribution a novel solver for temperature rate dependent crystallization processes in viscoelastic polymer melts is presented. It was composed in foam-extend-3.1 [1], a user community driven release of *OpenFOAM®*. The thermodynamic model for crystallization is a nonlinear source term of the energy equation depending on the temperature and its material time derivative as presented in [2]. Experimentally investigatable effects for this model are extensively described in [3]. A fluid-solid phase indicator is directly derived from the source term and used for mechanical modelling. For the fluid state stress is modelled by a Maxwell type of equation and to obtain a reliable solution the log-conformation reformulation [4] is applied. In the constitutive equation the fluid-solid transition is considered by parameter functions depending on the phase indicator and temperature. Solidified regions are excluded from the flow domain by manipulating the coefficient matrix of the momentum equation. The energy equation though, is solved for solidified regions.
Material modelling approaches, numerical implementation and results of a first study are presented. The focus regarding modelling is on the singular effects caused by solidification. Numerical aspects respectively coupling of fields and treatment of solidified regions are mentioned. The effectiveness of this approach is discussed on a simplified geometry for profile extrusion.

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S 9 : Laminar flows and transition

Tuesday 16:30 - 18:30 Marienstr. 13, 1st floor, Lecture hall D

Navier-Stokes computations versus interaction boundary layer theory results: a benchmark problem

S. Braun (TU Wien, Institute of Fluid Mechanics and Heat Transfer), T. Danczul (TU Wien, Institute of Analysis and Scientific Computing), P. Lederer (TU Wien, Institute of Analysis and Scientific Computing), M. Neunteufel (TU Wien, Institute of Analysis and Scientific Computing), J. Schöberl (TU Wien, Institute of Analysis and Scientific Computing) 16:30

Consider planar, incompressible laminar high Reynolds number (Re) flow between two parallel plates: fluid is removed through the permeable upper wall in order to generate adverse pressure gradient conditions in mean flow direction. As a consequence of relatively weak suction, the boundary layer at the impermeable lower wall is forced to separate locally. The corresponding reverse flow region (separation bubble) is known to react very sensitively to perturbations of any kind and typically undergoes rapid transition to the turbulent flow state. The present paper addresses a comparison between predictions of viscous-inviscid interaction boundary layer theory valid for $Re \to \infty$ and Navier–Stokes computations at finite, but high Re with regard to non-unique steady state solutions and an associated maximum, Re-dependent, value of the suction rate control parameter. To this end, a curve tracing algorithm is implemented into the hybrid discontinuous Galerkin method for the solution of the Navier–Stokes equations.

Measurements of partially lubricated contacts on different scales

M. Müller (Technische Universität Braunschweig), G. Ostermeyer (Technische Universität Braunschweig) 16:50

Tribological scenarios with partially filled gaps can occur when either a lubricated system runs under starved lubrication or a system that usually operates under dry conditions is wetted by a fluid. For several applications, a detailed experimental characterization of the corresponding transition regime from boundary lubrication to mixed lubrication has discovered a complex behavior of the friction coefficient and the wear rate with varying loading conditions, also known as Neo-Stribeck-curve.

Apart from specific applications, getting a fundamental understanding of such contact type is absolutely relevant, as it is present in numerous systems but not yet sufficiently comprehended. In order to get a detailed insight into the tribological character of partially filed gaps, it is necessary to investigate the dynamics of the fluid flow and its interaction with the pressure, velocity, nominal gap height and deformations.

Within this problem, the total amount of fluid in the gap plays a crucial role. Recent studies with novel models have shown that particularly near the fully filled regime the built up pressure is highly dependent of the filling ratio. Further studies proved that the fluid forms characteristic bow waves in front of asperities thus leading to larger mean

pressure values in the contact.
This paper focuses on experimental investigations for this contact type. The measurements are performed in two different scales. A pin-on-disc test bench represents the microscopic scale whereas a novel test bench with asperities in the range of centimeters corresponds to a rather macroscopic scale. The results are compared and conclusions towards the tribological properties are drawn.

Thermomagnetic convection under alternating magnetic fields

P. Szabo (Heriot-Watt University), W. Früh (Heriot-Watt University) 17:10

A parametric study was carried out to investigate the effect of alternating magnetic field on magnetic fluid to induce thermomagnetic convection. An external magnetic field with constant gradient and a set of alternating frequencies was used to investigate flow patters within a mineral oil base magnetic fluid by numerical simulations. All frequencies investigated alternated around a zero mean value starting from 0.5 to 2 Hz with an amplitude of 1×10^6 A/m. Transient changes in the magnetisation due to Néel relaxation and Brownian motion were neglect as they are several orders slower than the frequencies of the imposed magnetic fields.
As buoyancy is not present in this system the active driving force relates to the applied external magnetic field and is the Kelvin force. As the Curie law states that magnetisation is inversely proportional to temperature a net acceleration of colder, and therefore more magnetised, fluid in the direction of the applied magnetic field gradient is observed. The thermoconvective flow induced by the alternating magnetic field developed flow patterns of cold fluid towards higher magnetic field intensity with the frequency of that of the magnitude of the applied field but with varying amplitude.
A magnetic Rayleigh number analogous to the conventional Rayleigh number was defined to get an indication of the time-varying thermomagnetic convection. The response of the fluid was characterised by the Nusselt number, and it was found that the convection alternated with the frequency of that of the applied magnetic field which was reflected in the velocity and temperature profile of the magnetic fluid. The potential of thermomagnetic convection may be used for efficient cooling in heat transfer applications or in low-gravity environment where natural convection is not present.

Investigation of stress-velocity LSFEMs for the incompressible Navier-Stokes equations.

C. Nisters (Institute of Mechanics, University of Duisburg-Essen), A. Schwarz (Institute of Mechanics, University of Duisburg-Essen), J. Schröder (Institute of Mechanics, University of Duisburg-Essen) 17:30

In this contribution three mixed least-squares finite element methods (LSFEMs) for the incompressible Navier-Stokes equations are investigated with respect to accuracy and efficiency. The well-known stress-velocity-pressure formulation is the basis for two further div-grad least-squares formulations in terms of stresses and velocities (SV). Advantage of the SV formulations is a smaller system matrices size due to a reduction of the degrees

of freedom.
The least-squares finite element formulations, which are investigated in this contribution, base on the incompressible stationary Navier-Stokes equations consisting of the balance of momentum and the continuity equations. The first formulation to consider is the stress-velocity-pressure formulation according to [5]. Therefore, the Cauchy stress tensor $\boldsymbol{\sigma}$ is introduced as an additional variable to the system of equations. Secondly, a so-called (over-)constrained stress-velocity formulation is derived based on the findings in [5] and [2]. The expression *(over-)constrained* implies that a redundant residual is added to the functional without additional variables in order to strengthen specific physical relations, see e.g. [3]. The third formulation is a condensed stress-velocity formulation. Therefore, the pressure is interpolated discontinuously, and condensed on the discrete level without the need for any matrix inverting or storage of history variables.
The modified lid-driven cavity boundary value problem, which is a slight variant of the well-known lid-driven cavity problem, is investigated for the Reynolds numbers $Re = 400$ and $Re = 1000$ for all three formulations.

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Weakly nonlinear instability of a viscous liquid jet

G. Brenn (Graz University of Technology), M. Renoult (Université de Rouen), I. Mutabazi (Université du Havre) 17:50

The weakly nonlinear temporal instability of an axisymmetric Newtonian liquid jet is analysed. The first study on the nonlinear temporal capillary instability of a jet (J. Fluid Mech. 33 (1968), 151-163) was carried out for inviscid liquid and carried up to the third-order contribution to the jet deformation. A subsequent study showed that the inviscid weakly nonlinear theory is able to predict adequately the formation of satellite droplets in the capillary jet breakup (Phys. Fluids 18 (1975), 428-432). Here, the weakly nonlinear instability of a Newtonian liquid jet is examined as the viscous counterpart of the case studied before, in search for corresponding insight into the role of the liquid viscosity in the jet instability mechanism as achieved for viscous liquid sheets in (J. Fluid Mech. 735 (2013), 249-287).
We assume the jet liquid to be incompressible and Newtonian. The problem is formulated in cylindrical coordinates. Body forces are neglected, since the Froude number is large. The governing equations are non-dimensionalized with the undeformed jet radius a, the

time scale $(\rho a^3/\sigma)^{1/2}$ and the pressure σ/a, where ρ is the liquid density and σ the liquid-air surface tension. The equations of motion are linearised, formulating velocities and pressure as consequences of small deformations of the jet surface. Representing the velocities as derivatives of a disturbance stream function and taking the curl of the momentum equation, a fourth-order partial differential equation governing the disturbance stream function is obtained. Its solution reads

$$\psi(r,z,t) = (C_1 r I_1(kr) + C_3 r I_1(lr))\, exp(ikz - \alpha_1 t) \ ,$$

where k is the real disturbance wave number, α_1 is a disturbance growth rate, and I_1 is a modified Bessel function of the first kind. We have discarded the modified Bessel functions of the second kind for regularity of the solution on the jet axis. We have furthermore defined $l^2 = k^2 - \alpha_1/Oh$ and the Ohnesorge number $Oh = \mu/(\sigma a \rho)^{1/2}$, where μ is the liquid dynamic viscosity. The flow field is determined by spatial derivatives of the stream function, and the two integration constants are determined by the kinematic and dynamic, zero-shear stress boundary conditions. The normal-stress boundary condition yields the dispersion relation governing the linear stability behaviour of the jet. The nonlinear behaviour is now obtained by representing the velocity components and the pressure by series expansions with a small parameter η_0 corresponding to the initial deformation amplitude. The expansion for the axial flow velocity, as an example, reads

$$u_z = u_{z1}\eta_0 + u_{z2}\eta_0^2 + \dots \ .$$

Introducing the expansions into the equations of motion and the boundary conditions, we obtain equations determining the linear problem in terms of the quantities with subscript 1, and the second-order problem by quantities with subscript 2. The related equations are linear in the quantities of the respective order, but non-linear in the quantities of the next lower order. Solving the equations for the second order for inviscid jet liquid yields the results of (J. Fluid Mech. 33 (1968), 151-163), with two typographical corrections. Accounting for the jet liquid viscosity, the second-order pressure field is governed by a Poisson equation with a right-hand side consisting of products of modified Bessel functions. The particular solution of the inhomogeneous equation is searched for in a form containing the solution for the inviscid case in a closed form and for the viscous case in a polynomial approximation. The resulting velocity and pressure fields, as well as the jet surface shape, are evaluated for given jet Ohnesorge numbers. The jet surface shape shows the influence from the nonlinear interaction of the first and second orders. Evaluating the influence of the liquid dynamic viscosity on the instability behaviour of the jet reveals the dependency of the jet behaviour on both the Oh number and the wave number k of the disturbance.

S 10: Turbulence and reactive flows

Organizers: Martin Oberlack (TU Darmstadt)
Jörg Schumacher (TU Ilmenau, Fak. Maschinenbau)

S 10 : Turbulence and reactive flows

Thursday 14:00 - 16:00 Marienstr. 7, 2nd floor, Room 206
Chair: Jörg Schumacher (TU Ilmenau)
Martin Oberlack (TU Darmstadt)

Physics of rotating fluids, a DFG core facility centre

S. Merbold (BTU Cottbus - Senftenberg), U. Harlander (BTU Cottbus - Senftenberg), C. Egbers (BTU Cottbus - Senftenberg) 14:00

The present project aims to establish a new international research center (core facility center) for "Physics of Rotating Fluids (PRF)" with geo-/astrophysical, meteorological and technical applications located at Brandenburg University of Technology Cottbus-Senftenberg. The main goal is to integrate cutting-edge rotating and stratified fluid flow experiments across national boundaries in order to foster internationally competitive experimental research in the field of rotating and stratified fluids by providing an easy access to experimental facilities equipped with state-of-the-art instrumentation.
The research areas covered by the experimental facilities inside the new center are: Planetary and astrophysical flows (with focus on disk formation, instabilities and mixing), Geophysical fluid dynamics (with focus on strato-rotational turbulence, mean flow generation and wave interaction) as well as Rotating flows with technical applications (centrifuges, turbines, journal bearings and rotor/stator cavities). The new center of "Physics of Rotating Fluids (PRF)" will cover and focus all previous single research and guest scientist exchange activities like EUHIT, CNRS French/German-co-operation and ESA Topical Team with BTU/CFTM^2 in the field of rotating and stratified fluid flows.
As an example of the performance of the Core Facility Centre we briefly present research on the classical Taylor-Couette problem but in the limit of very wide gaps (radius ratio smaller than 0.5), while both cylinders rotate at different speeds. This geometry is less investigated compared to narrow gaps [Grossmann et al., Annu. Rev. Fluid. Mech. 48, 53–80, 2016] and reveals a huge number of flow instabilities and transport phenomena. We discuss the flow structures and their contribution to the torque needed to rotate the cylinders at constant speed.
Funding by DFG under grant EG100/23-1 and HA2932/10-1 is gratefully acknowledged.

CFD studies on the surge detection of a radial compressor flow by analyzing the unsteady secondary flow field

S. Bamberg (Hochschule RheinMain), J. Schnitzer (Technische Universität Ilmenau), M. Weber (Hochschule RheinMain), S. Rusche (Hochschule RheinMain), W. Eißler (Technische Universität Ilmenau) 14:20

In consequence of the worldwide scarcity of fossil resources and the climate change, induced by the excessive CO_2 emissions, mankind has to handle the remaining stocks sustainable and thrifty. To safe fuel and to minimize emissions, modern combustion engines are typically equipped with turbocharger compressors which increases the air mass for the combustion process. Thus the specific performance of the engine is improved so that smaller engines with an equal performance range can be realized. [4] Generally centrifugal compressors are used for automotive turbochargers. [3] Due to the so called compressor surge occurring at low air mass flow rates the stable operating range is limited. This limitation is indicated by the surge line in the performance map. [1] The overall aim for any new developed compressor is the expansion of the stable operating range by shifting the surge line to lower air flows. It is already known that mixed flow centrifugal pumps are more resistant to this negative effect resulting in a more stable head curve. [2] Designing a mixed flow compressor wheel with advanced properties might increase the stable operating range.

The objective of this investigation is the development of a reliable methodology allowing the accurate prediction of the characteristic operating map supporting the designing process. In this context a centrifugal compressor used in a commercial application with five main and five splitter blades, installed in regular passenger vehicles, is numerically analyzed. For this purpose a CFD analysis is conducted.

On the one hand a full model consisting of the whole impeller as well as the volute and on the other hand only one blade passage with one main and one splitter blade is considered. Steady-state simulations for both models and unsteady simulations for the sector model are performed with a constant number of revolutions and a varying air mass flow rate using the RANS methodology. The numerical results of the full model are validated with an existing operating map which was experimentally determined on a test rig and coincide well with the reality within a wide range. Based on the missing volute, the outcome of the sector model is compared with the full model at defined locations in the fluid domain. Opposing the results of both models it becomes apparent that there is a good accordance in the qualitative run of the stream. To understand the initiation of surge more profoundly, the numerical results of the steady and unsteady simulations are analyzed to detect the onset of fluctuations in the flow field as shown in figure 1.

Moreover the flow field is studied by contour as well as vector plots, streamlines, etc. to visualize the global backflow induced by the compressor surge and local stall due to different operating points. Besides this, secondary flows, especially three-dimensional coherent turbulent structures in the form of vortices, are examined and depicted on isosurfaces by applying different vortex detection criteria, like the Q- or the λ_2-criterion.

Keywords: CFD, turbocharger, centrifugal compressor, surge line, secondary flow, co-

herent structures

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Optimal quadric parametrization of the lattice Boltzmann method

M. Geier (TU-Braunschweig), A. Pasquali, M. Schönherr 14:40

It was proposed more than 20 years ago by Ginzburg and Adler [Ginburg and Adler J. Phys. II 4 (2) 1994] that the accuracy order of the lattice Boltzmann method for fluid flow can be raised to fourth order by the utilization of so-call magic collision numbers. Their method, that received several reviews in the past two decades, was of mixed success. Even though the error could be controlled, the parameterization turned out to be case dependent such that no real fourth order accuracy could be obtained. In this contribution we show that the cancelation of the leading error in diffusion imposes five independent constraints that requires the selection of five independent magic parameters. The original proposal of Ginzburg et al. had only one parameter and could hence not solve the problem in the general case. We propose to use a cumulant decomposition of the momentum distribution function that gives us three independent free collision rates to control the error. By modifying the equilibrium cumulants we are able to obtain two more free parameters that allow us to solve the system in the general case. That is, there exists one unique solution for the parametrization of the cumulant lattice Boltzmann method that eliminates the leading order error in the diffusion completely and independently of the flow. We demonstrate the fidelity of the optimized cumulant method with the direct simulation of the drag crisis emerging in the flow over a sphere at Reynolds numbers in the range of 10^5 to 10^6.

On Turbulent Scalar Transport at Very High Schmidt Numbers Using a Stochastic Modeling Approach

M. Klein (BTU Cottbus - Senftenberg), H. Schmidt (BTU Cottbus - Senftenberg) 15:00

Understanding turbulent transport of passive scalars (like mass or temperature) is relevant for many practical applications, for example for correct modeling of the cooling rates in an industrial device. The transport of scalars with low diffusivity (high Schmidt

number) has remained inaccessible to direct numerical simulations (DNS) or large-eddy simulations (LES) due to the resolution requirements. Instead, asymptotic theory has been used to predict the scalar mass transfer at high Schmidt numbers. We aim to asses the theory used by studying the scalar transport in fully-developed channel flows at Schmidt numbers up to $Sc \sim 10^4$ using a stochastic turbulence model, the so-called one-dimensional turbulence (ODT). The channel flow is driven by an imposed pressure gradient, homogeneous no-slip conditions apply at the walls and the scalar is injected by Dirichlet boundary conditions at the walls.
In this study we use ODT as stand-alone tool to make high-Schmidt number simulations feasible. ODT aims to reproduce the statistics of a 3-D turbulent flow on a 1-D domain. Channel flow profiles are thus obtained by integrating a set of stochastically perturbed partial differential equations in time. The stochastic perturbations, so-called eddy events, model the turbulent advection. Eddy events are sampled from an eddy probability density function (eddy PDF) which depends on the flow state. Implemented eddies modify the flow state and, hence, the eddy PDF so that a feedback mechanism is established which aims to mimic the kinematics of Navier–Stokes turbulence. In order to avoid expensive construction of the eddy PDF at each time step sampling from an approximate PDF is used in conjunction with a thinning and rejection algorithm. Eddy events are implemented by triplet mapping the velocity and scalar profiles within the eddy region. The triplet map models phenomenologically the turbulent stirring induced by a physical eddy and can be computed efficiently.
In our talk we will discuss statistics of the velocity components and the passive scalar by comparing ODT results to DNS data. Emphasize will be put on the scalar mass transfer at high Schmidt numbers, where ODT results will be compared to asymptotic theory for various Reynolds numbers ($10^2 < Re_\tau < 10^4$). Good qualitative and quantitative agreement has been obtained between ODT, DNS and asymptotic theory. Preliminary results suggest that the scalar mass transfer scaling exponent might need a correction at high Schmidt numbers.

Heat and momentum transfer for magnetoconvection in a vertical external magnetic field

T. Zürner (TU Ilmenau), W. Liu (TU Ilmenau), D. Krasnov (TU Ilmenau), J. Schumacher (TU Ilmenau) 15:20

The scaling theory of Grossmann and Lohse (J. Fluid Mech. 407, 27 (2000)) for the turbulent heat and momentum transfer is extended to the magnetoconvection case in the presence of a (strong) vertical magnetic field. The comparison with existing laboratory experiments and direct numerical simulations in the quasistatic limit allows to restrict the parameter space to very low Prandtl and magnetic Prandtl numbers and thus to reduce the number of unknown parameters in the model. Also included is the Chandrasekhar limit for which the outer magnetic induction field **B** is large enough such that convective motion is suppressed and heat is transported by diffusion. Our theory identifies four distinct regimes of magnetoconvection which are distinguished by the strength of the outer magnetic field and the level of turbulence in the flow, respectively.

S 10 : Turbulence and reactive flows

Thursday 16:30 - 18:30 Marienstr. 7, 2nd floor, Room 206
Chair: Martin Oberlack (TU Darmstadt)

Evaluating flame turbulence scale in diffusion combustion of diesel fuels

O. Matvienko (National Research Tomsk State University), E. Loboda (National Research Tomsk State University), M. Agafontsev (National Research Tomsk State University), V. Reyno (Institute of Atmospheric Optics Russian by V.E. Zuyev, Russian Academy of Science) 16:30

Diffusion burning occurs in the flames from both mechanical burners and natural fires when the combustion products exhibit turbulent flow [1]. Although turbulent burning has been studied by many researchers [2-6], a detailed description of this phenomenon remains a challenge. Many aspects of this problem have not been explored either theoretically or experimentally, and even a plan to complete the technical tasks required to understand the processes has not yet been formulated. The authors believe that many aspects of turbulent flame combustion can be thoroughly studied by using remote sensing techniques including IR thermography.

Flame turbulence scale can be experimentally evaluated by analyzing IR thermograms of flame jets obtained in narrow spectral bands corresponding to the spectra of some marker gases (water vapor and CO_2), as shown in [7]. In the same research, by assuming the similarity of pulsations of hydro- and thermo-dynamic parameters, the relationship between turbulence scale and characteristic frequencies of temperature pulsations in flames was mathematically investigated.

In this paper, we propose a mathematical model of diesel fuel combustion and compare the theoretical results with the experimental results obtained by thermographically estimating the size of temperature non-homogeneities and turbulence scale. Methodical aspects of this research were reported in [7].

Acknowledgements:
This research was supported by grant № 15-01-00513 from the Russian Fund for Fundamental Research .

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Application of ODT to constant volume autoignition problems

J. Medina (BTU Cottbus), H. Schmidt (BTU Cottbus) 16:50

The One-Dimensional Turbulence (ODT) model is applied to a constant volume configuration by means of a periodic, one-dimensional domain subject to randomized ensemble members with initial inhomogeneous temperature fields and homogeneous mass fraction profiles. The multidimensional turbulent interactions in the flow are modeled by the separate implementation of turbulent advection and the diffusion-reaction processes, neglecting the mean advection of the system. On one hand, turbulent advection is modeled by means of the eddy events defined within the framework of ODT; on the other hand, the diffusion-reaction system is solved by means of the Zero-Mach limit conservation equations discretized with a 1D Finite Volume Method. Unlike previous studies for constant volume autoignition flows done with similar ODT-frameworks, an extended algorithm for the Zero-Mach limit approximation in constant volume systems is proposed in this work in order to fulfill the simultaneous advancement of the continuity equation, ideal gas law and diffusion-reaction evolution equations for the enthalpy and mass fractions. Due to the inherent stiffness of the diffusion-reaction system, an operator splitting approach is also included in the formulation.
Results for n-Heptane chemistry comprising the temporal evolution of the heat release rate, pressure and density-weighted displacement speed are shown and compared to DNS results from Yoo et al. [Combust. Flame 158 (2011) 1727-1741] in terms of individual ensemble members and mean ensemble behavior. Additionally, a brief sensitivity analysis of the reaction chemistry is performed by means of the variation of the applied chemical reaction mechanism.
Overall, this work presents the framework for constant volume autoignition in ODT and shows its efficiency for complex chemistry simulations.

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S 10 : Turbulence and reactive flows

Friday 09:00 - 11:00 Marienstr. 7, 2nd floor, Room 206
Chair: Jörg Schumacher (TU Ilmenau)

Investigating Asymptotic Suction Boundary Layers using a One-Dimensional Stochastic Turbulence Model

M. Fragner (BTU Cottbus - Senftenberg), H. Schmidt (BTU Cottbus - Senftenberg) 09:00

In the talk we will summarize the results described in a recent article (submitted to Journal of Turbulence) in which the turbulent asymptotic suction boundary layer is studied using a one-dimensional turbulence (ODT) model. ODT is a fully resolved, unsteady stochastic simulation technique. While flow properties reside on a one-dimensional domain, turbulent advection is represented using mapping events whose occurrences are governed by a random process. Due its reduced spatial dimensionality ODT achieves major cost reductions compared to full 3D simulations, which allows simulations for a larger Reynolds number range than currently accessible via DNS or even LES. A quantitative comparison to recent DNS data at moderate Reynolds number ($Re = u_\infty/v_0 = 333$, where u_∞ and v_0 are the free stream and suction velocity, respectively) suggests that the ODT model has excellent capabilities in reproducing several velocity statistics, i.e. mean velocity, turbulent stresses and turbulent kinetic energy budgets. Variation of the

Reynolds number in the range $Re \in [333, 400, 500, 1000]$ shows that ODT can reproduce various physical phenomena that have been observed as a result of suction in turbulent boundary layers, i.e. the reduction of Reynolds stresses, increased anisotropy near the wall and enhanced skin friction and turbulent friction Reynolds numbers Re_τ. Presenting several local eddy size distributions, we show that the reduction of Reynolds stresses near the wall correlates with a suppression of larger eddies further away from the wall when suction is introduced. While up to $Re = 500$ our results can be directly compared to recent LES data, the simulation at $Re = 1000$ is currently not feasible through full 3D simulations. This demonstrates the potential of the ODT methodology to assist in the design process of possible future DNS simulations on suction boundary layers.

Scaling laws for velocity and temperature in the near-wall region of compressible turbulent boundary layers

I. Vigdorovich (Lomonosov Moscow State University) 09:20

Scaling laws for velocity and temperature profiles in the near-wall region of sub- and supersonic turbulent boundary layers have been developed, which allow us to represent velocity and temperature profiles in compressible gas stream in terms of those in an incompressible boundary layer. They are obtained as asymptotic expansions of the solutions to the Reynolds equations in a small parameter — the Mach number based on the friction velocity and gas enthalpy on the wall. The leading term of the expansion for velocity corresponds to known Van Driest's formula. However, the obtained solution contains additional terms of order unity, which explains the contradiction between Van Driest's formula and experimental data. The law of the wall for temperature, which has been formulated for the first time, has an analogous structure. Besides the von Kármán constant and the turbulent Prandtl number in the logarithmic region, known for incompressible flow, the obtained relations contain three new universal constants, which do not depend on gas molecular properties and specific heat ratio.

Flow organization in the region of the torque maximum in a wide gap Tayor-Couette experiment

A. Froitzheim (BTU Cottbus - Senftenberg), S. Merbold (BTU Cottbus - Senftenberg), C. Egbers (BTU Cottbus - Senftenberg) 09:40

The flow in the gap enclosed by two independently rotating cylinders and two end plates is called Taylor-Couette flow (TC). Due to the rich dynamic behavior of this system many different flow states can be realized by adjusting the control parameters radius ratio $\eta = r_1/r_2$, aspect ratio $\Gamma = L/d$, the ratio of angular velocities $\mu = \omega_2/\omega_1$ and the shear Reynolds number $Re_S = 2r_1r_2d|\omega_2 - \omega_1|/(\nu(r_1 + r_2))$ with the kinematic ν, the gap width $d = r_2 - r_1$ and the indices 1 and 2 for the inner and outer cylinder respectively.

Our study is focused on a wide gap TC experiment ($\eta = 0.5$), as most of the existing numerical and experimental investigations were done in small gap geometries ($\eta > 0.71$) [3]. When the radius ratio is decreased the curvature of the cylinders gain importance,

which leads to a considerable difference in the boundary layer thicknesses at the inner and outer cylinder [2]. Further, the transport of angular momentum J_ω exhibits a maximum in the low counter-rotating regime and its location is predicted to shift towards pure inner cylinder rotation when η is decreased [1]. Up to now the reason for this maximum and its change in the wide gap configuration is an actual research topic and will be investigated within this study.

For our investigations we will use the Top-view-Taylor-Couette-Cottbus experiment with $r_1 = 35\,mm$, $r_2 = 70\,mm$ and $L = 700\,mm$ leading to $\eta = 0.5$, $\Gamma = 20$ and $d = 35\,mm$. 2D2C-PIV measurements will be done in horizontal planes at different heights to investigate the flow field in the region of the torque maximum ($\mu_{max}(\eta = 0.5) = -0.2$, [4]) at different shear Reynolds numbers in the range of $4 \cdot 10^4 \leq Re_S \leq 2 \cdot 10^5$. We try to get a better understanding of the influence of the rotation ratio μ on the flow state and especially on the reasons for μ_{max}.

We gratefully acknowledge financial funding by the DFG FOR 1182 (EG 100/15-1, 15-2).

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T-mixer an novel system to investigate decaying turbulence in a wall-bounded environment

T. Schikarski, M. Avila (Chair of Fluid Mechanics) 10:00

The universality of decaying homogeneous isotropic turbulence (HIT) with a power law is accepted in the turbulence community, but remains an unsolved and controversially discussed question for wall-bounded flows. More precisely, only a few studies [**?**, **?**] considered the decay process in a wall-bounded domain. The former introduced the wall effects by applying a low-wavenumber cut-off into energy spectrum of isotropic turbulence. By doing so, they found that the power law is preserved with resulting exponents consistent to those of HIT. The latter studied experimentally the decay of high- Reynolds number Taylor-Couette turbulence by removing the energy input with stopping the inner cylinder. Controversially, Verschoof *et al.* [**?**] state that the decay

process doesn't follow a strict power law, but it is faster, due the viscous drag of the bounding walls.
Our first analyses indicate that a simple T-mixer is an ideal system to investigate decaying turbulence in wall-bounded flows. The colliding inlet streams generate turbulence at the junction, which diminishes by shear along the outlet [**?**]. Surprisingly, at the center line of the mixing channel the decay of turbulent kinetic energy k and its counterpart $\langle \phi' \phi' \rangle$ for a passive scalar follows strictly a power law with a Reynolds number independent exponent. The value of each exponent agrees very well with those found by HIT experiments, theoretical works and simulations [**?**, **?**, **?**]. More precisely, the turbulent kinetic energy decays as $k \propto a(Re)y^{-2}$. Similar to k, the scalar variance follows a power law $\langle \phi' \phi' \rangle \propto b(Re)y^{-1.4}$ in agreement with [**?**]. We will show the influence of the evolving anisotropy apart from the center line on the decay process, which contributes to this fundamental and controversially discussed topic.

A Lagrangian tracking of energetic motions in fully developed turbulent pipe flow

A. Shahirpour (BTU Cottbus - Senftenberg), J. Sesterhenn (TU Berlin), C. Egbers (BTU Cottbus - Senftenberg) 10:20

Coherent structures are known as organized motions which posses coherence in space and time being defined as entities which stay observable while evolving in space and changing moderately within a certain time span. Given the transport-dominated nature of structures in wall bounded turbulent flows, standard decomposition methods like Dynamic Mode Decomposition (DMD) will fail to reconstruct a reduced-order model of the flow with a minimal number of modes. Using a Lagrangian DMD instead (Sesterhenn & Shahirpour), the structures will be followed in a properly chosen frame of reference along the characteristics which represent the convective velocity of the structure to be captured. In the present study this method is applied to existing DNS of fully developed turbulent pipe flow at bulk Reynolds number of $Re_b = 25 \times 10^3$, aiming at capturing energetic motions in such flows.
The latter will take place using a coordinate transformation from physical space into spatio-temporal space. The transformation will be in form of a rotation in space and time with the rotation angle corresponding to the most dominant group velocity u_g in the flow, determined by the maximum drop of the singular values. The transformed snapshots will be decomposed using the standard DMD algorithm (Schmid and Sesterhenn 2008). In the final step, the dynamic modes being reconstructed in the spatio temporal space will be transformed back to physical space. The latter will represent a reduced order model of the system using only a few modes accommodating the structure with the dominant group velocity.
To follow the footprints of large-scale energetic motions, it is common practice to observe the velocity spectrum and premultiplied velocity spectrum which represent the energy content of the flow in the wavenumber space. In order to examine the captured dynamic modes, a similar approach is adopted for single and summed up $\mathcal{L}$DMD modes, and compared against the full-field spectra. This comparative analysis shows that the

first few $\mathcal{L}$DMD modes, (when sorted by their decay rate in ascending order), posses maximum energy content, at wave lengths corresponding to that of the outer spectral peak of the full-field. In other words, only a few modes that have small decay rates are required, to encapsulate the structures with maximum energy while accommodating only a few wavelengths. The energy content of these modes, when summed up, builds up to a magnitude close to the maximum energy content of the full-field. As validations prove, the reduced order model reconstructed using the $\mathcal{L}$DMD modes, represents a higher energy level with fewer modes in comparison with the standard DMD results, hence providing a better means of understanding the dynamics of such structures as well as their contribution to turbulent properties like Reynolds stress tensor.

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[2] P. J. Schmid, J. Sesterhenn, *Dynamic mode decomposition of numerical and experimental data,* 61st Annual Meeting of the APS Division of Fluid Dynamics, San Antonio, Texas, November 2008.

S 11: Interfacial flows

Organizers: Jochen Fröhlich (TU Dresden)
Michael Manhart (TU München)

S 11 : Interfacial flows

Thursday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 104
Chair: Jochen Fröhlich (TU Dresden)

Discontinuous Galerkin Methods for fluid dynamical problems with dynamic boundaries: multiphase flows

M. Oberlack (TU Darmstadt), F. Kummer (TU Darmstadt), B. Müller (TU Darmstadt), T. Utz (TU Darmstadt), M. Smuda (TU Darmstadt) 14:00

Discontinuous Galerkin (DG) methods can be constructed for arbitrary convergence orders if the solution to the continuous problem is sufficiently smooth. This assumption does not hold for multiphase flows, which are mixtures of two or more immiscible fluids with different density and viscosity and also depend on surface tension effects. In such flows, the pressure and the velocity gradient are discontinuous at the fluid interface. Any high-order method applied to this problem requires a special treatment of this singularity in order to obtain its designed performance. We are going to present a DG discretization for multiphase flow problems, which employs an adaption of the approximation space

("cut cells") in each time-step to the position of the fluid interface and is therefore able to achieve high convergence order. Since the shape and position of the interface can be almost arbitrary, one has to deal with difficulties like arbitrarily small cut cells. Furthermore, since the approximation space depends on time, one also has to adopt the temporal integration in order to deal with cut cell which change their shape over time. Within the past years, several building blocks of such a method were presented: this includes numerical integration on cut cells, precise evaluation of curvature and level-set algorithms to compute the evolution of the interface. In the integration of those blocks into a full multiphase-solver, one has to consider complex non-linear interactions, e.g. between the interface dynamics and the approximation space: the flow velocity determines the evolution of the fluid interface which then changes the approximation space. Therefore, the presentation will not only cover a short review of the individual building blocks but will also discuss several pitfalls which may occur in the combination of these blocks.

Acknowledgements:
The work of F. Kummer is supported by the German Research Foundation (DFG) through the Collaborative Research Center 1194/B06. The work of B. Müller is supported by the German Research Foundation (DFG) through Research Grant WA 2610/2-1. The work of T. Utz is supported by the German Research Foundation (DFG) through the Priority Programme 1506. The work of M. Smuda is supported by the German Research Foundation (DFG) through the Graduate School of Computational Engineering.

Coupling of topology, geometry and dynamics in a surface Navier-Stokes equation

A. Voigt 14:20

We consider a numerical approach for the incompressible surface Navier-Stokes equation. The approach is based on the covariant form and uses discrete exterior calculus (DEC) in space and a semi-implicit discretization in time. The discretization is described in detail and related to finite difference schemes on staggered grids in flat space for which we demonstrate second order convergence. We compare computational results with a vorticity-stream function approach for surfaces with genus g(S) = 0 and demonstrate the interplay between topology, geometry and flow properties. Our discretization also allows to handle harmonic vector fields, which we demonstrate on a torus.

Numerical modeling of shockwaves in biomedicine

S. Adami (TU München), J. Kaiser, N. Adams 14:40

We have developed a multi-phase compressible fluid solver that can handle shockwaves efficiently and accurately. Using a level set formulation to treat sharp interfaces and employing multi-resolution techniques, we can study complex shock-bubble interactions. In this work, shock-induced bubble collapse interactions near a deformable interface are presented as a model for a simplified extracorporeal shockwave lithotripsy experiment.

The conservative sharp-interface method was successfully validated for free-field collapse and non-spherical collapse near solid walls. We observe a systematic small deviation of our results compared with that of the diffuse-interface method from the literature.

On fluid interfaces and phase connectivity during viscous-dominated primary drainage

R. Sivanesapillai (University of Stuttgart), H. Steeb (University of Stuttgart) 15:00

We perform pore-scale resolved direct numerical simulations of immiscible two-phase flow in porous media to analyze the mechanisms by means of which discrete fluid-fluid interfaces evolve. While pore-scale imaging methods, e.g. fast X-ray tomography methods, to study the distribution and evolution of fluid-fluid interfaces for capillary-dominated flow become increasingly mature [1,2], their applicability to viscous-dominated flow is limited by temporal resolution. We consider hydrodynamic direct numerical simulations (DNS) a suitable complementary approach to study viscous-dominated two-phase flow. Using a Smoothed-Particle Hydrodynamics model [3], we present DNS of primary drainage in partially wettable 2D porous media of particulate microstructure at large capillary numbers.

During viscous fingering, pore-scale flow fields are reminiscent of Bretherton annular flow, i.e. the less viscous phase percolates through the core of a pore-throat forming a hydrodynamic wetting film. Even in simple microstructures, wetting films are shown to have major impact on the evolution of fluid-fluid interfacial area and to give rise to non-negligible interfacial viscous coupling.

Recently, Schlüter et. al. (2016) demonstrated the fundamental role of fluid topology in permanent hysteresis effects during drainage and imbibition. A topological analysis of wetting phase connectivity during primary drainage thus emphasizes on topological implications of 2D simulations. In contrast to viscous fingering in 3D porous structures, Bretherton flow in 2D porous media is shown to result in the isolation of wetting films. Finally, we discuss future applications of SPH to model two-phase flow in 3D porous media using image-based data.

[1] Wildenschild, D., and A. P. Sheppard (2013), X-ray imaging and analysis techniques for quantifying pore-scale structure and processes in subsurface porous medium systems, *Adv. Water Resour.*, *51*, 2013, doi:10.1016/j.advwatres.2012.07.018.

[2] Schlüter, S., S. Berg, M. Rücker, R. T. Armstrong, H.-J. Vogel, R. Hilfer, and D. Wildenschild (2016), Pore-scale displacement mechanisms as a source of hysteresis for two-phase flow in porous media, *Water Resour. Res.*, *52*(3), 2016, doi:10.1002/2015WR018254.

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Numerical investigation into a liquid displacing a gas in thin porous layers

T. Neumann (TU Dortmund), P. Ehrhard (TU Dortmund), K. Boettcher (TU Dortmund) 15:20

Lithium-ion batteries are composed of several single cells, each consisting of conductive, impermeable electrodes made of aluminum and copper. Both are coated with a thin, porous layer on both sides of the electrode (collectors) and a thin, non-conductive and permeable layer is separating them. To estimate the filling process of these batteries with an electrolyte, a numerical model for the flow of a well-wetting liquid displacing a gas in a single cell is established. Related to this problem, a single cell can be modelled as a stack of three porous layers with heterogeneous characteristics. The porous structure of the electrode coatings is approximated as a packed bed of spheres. Considering the small ratio of layer thickness to particle diameter, the influence of the wall effect onto the relevant forces has to be taken into account.

The characterization of this flow is based upon volume-averaged parameters; models describing the relevant forces according to the hydrodynamics of this multi-phase flow are implemented into the commercial CFD-software Ansys CFX. With respect to the regularity in the arrangement of the spheres near the plain wall of the electrodes, the local dependence of the porosity $\varepsilon(z)$ on the wall distance z is considered. Theoretical models are used to determine a correlation between $\varepsilon(z)$ and the hydraulic diameter $d_h(z)$, which provides a measure for the pore diameter. For the filling process, small Reynolds numbers are expected so that inertial forces can be neglected. The implemented viscous and capillary forces depend on $d_h(z)$ which allows a local resolution of the two-phase flow with respect to z. Friction at the electrode is taken into account, while the contact line is allowed to move along the wall. The influence of capillary forces at the plain wall is implemented separately.

The implementation of the forces is validated against the analytical solution of a one-dimensional, capillary-driven flow in a homogenous porous medium without wall effect. Furthermore, results of the displacement flow in parts of the single cell are presented and discussed, showing a considerable influence of the modelled effects onto the flow characteristics.

Adaptive Temporal Refinement in Mold Filling Simulations

V. Karyofylli (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), L. Wendling (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), M. Frings (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), S. Elgeti (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), M. Behr (RWTH Aachen University, Chair for Computational Analysis of Technical Systems) 15:40

The aim of this talk is to highlight how the temporal refinement is applied in the vicinity of an evolving interface, by means of a space-time finite element discretization.

Space-time method has an inherent flexibility to admit completely unstructured meshes with varying levels of refinement not only in spatial dimensions, but also in the time dimension. 4D simplex-based space-time grids are used within the framework of this adaptive refinement and give us the flexibility to use a type of local time-stepping for our simulations. The method used for generating this type of meshes has been already described in [3].
We focus on mold filling which is an important stage of die-casting and injection moulding, the most commonly used manufacturing processes for producing metal, polymeric and ceramic components. As a consequence, the numerical simulation of this process based on computational fluid dynamics is of great significance for the production engineering [1]. However, modeling of the mold filling is a tremendously demanding process, because many complex physical phenomena, such as the two-phase flow, the propagation of an interface, the surface tension, etc., must be taken into account. Nevertheless, the efficiency of our simulations is improved when using local temporal refinement.
The governing equations for the two-phase flow during the filling stage are the transient, incompressible Navier-Stokes equations, since we assume that the fluids of our interest are incompressible and Newtonian. We use a stabilized finite element method in combination with space-time meshes in order to discretize them. For the description of the moving front, an interface capturing method based on the Eulerian formulation, such as the level-set method, is used, because of its inherent ability to account for topological changes of the interface [2]. The interface is described implicitly by the level-set field on a fixed mesh.
The numerical examples, used for validating the unstructured space-time mesh solver and the refinement scheme, involve the benchmark cases of a static drop inside a square domain, a rising bubble in a rectangular domain and the filling of mold cavities.

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S 11 : Interfacial flows

Thursday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 104
Chair: Kerstin Eckert (TU Dresden)

Attractors for the motion of finite-size particles in a two-sided lid-driven cavity

H. Wu (Institute of Fluid Mechanics and Heat Transfer, TU Wien), F. Romano (Institute of Fluid Mechanics and Heat Transfer, TU Wien), H. Kuhlmann (Institute of Fluid Mechanics and Heat Transfer, TU Wien) 16:30

Particle trajectories in an incompressible cavity flow driven by two facing walls moving in opposite directions are investigated experimentally. On an increase of the Reynolds number the flow in a two-sided lid-driven cavity with aspect ratio 1.7 bifurcates from a steady two-dimensional flow to a steady three-dimensional periodic cellular flow [1, 2]. In such a steady three-dimensional flow the whole volume is partitioned into regions of chaotic and of regular streamlines [3], the latter arising in form of Kolmogorov-Arnold-Moser tori. When finite-size and neutrally-buoyant particles are transported near boundaries, they experience strong forces due to the particle-boundary interaction [5]. The dissipative effect associated with this interaction causes a rapid attraction to a periodic or quasi-periodic attractor which is usually located inside a regular region of the flow [5]. Three-dimensional particle tracking is used to reconstruct a single particle trajectory. Furthermore, a statistical analysis has been made by repeating single-particle-tracking experiments with randomized initial particle positions. Experimental results and a comparison with numerical simulations will be presented and discussed.

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[2] S. Albensoeder and H. C. Kuhlmann. Linear stability of rectangular cavity flows driven by anti-parallel motion of two facing walls. *Journal of Fluid Mechanics*, 458:153–180, 2002.

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[4] F. Romanò and H. C. Kuhlmann. Numerical investigation of the interaction of a finite-size particle with a tangentially moving boundary. *International Journal of Heat and Fluid Flow*, 62PA:75–82, 2016.

[5] H. C. Kuhlmann, F. Romanò, H. Wu and S. Albensoeder. Particle-motion attractors due to particle-boundary interaction in incompressible steady three-dimensional cavity flow. In *20th Australasian Fluid Mechanics Conference*, book of abstracts p. 102, paper no. 449, 2016.

Tracking the translational and rotational motion of small ellipsoidal particles in lid-driven cavity flow

Y. Cui (Friedrich-Alexander-Universität Erlangen-Nürnberg), M. Hriberšek (University of Maribor), J. Ravnik (University of Maribor), P. Steinmann (Friedrich-Alexander-Universität Erlangen-Nürnberg) 16:50

In this work the Lagrangian particle tracking of small ellipsoidal particles with focus on its translational and rotational momentum transfer in a lid-driven cavity flow is studied. The particle motion is tracked in space solving for both the translational and the rotational motion whereby the orientation of the ellipsoidal particle is obtained through the Euler parameters. The time evolution of the Euler parameters is related to the angular velocity of the particle in the particle frame of reference, whereas the time evolution of angular velocity is related to the hydrodynamic torque acting on ellipsoidal particles. The drag force on ellipsoid with respect to the orientation angle can be derived by resistance tensor and rotation matrix, and the Saffman lift force for an ellipsoid can be calculated by employing a lift tensor. The described physical models were implemented into the open source software OpenFOAM®, which is now able to perform Lagrangian particle tracking of ellipsoidal particles. The developed simulation tool was used to simulate a dilute suspension of ellipsoidal particles in a lid driven cavity flow. The particle Stokes number, the cavity flow Reynolds number and ellipsoid aspect ratio were varied to encompass the different regimes of interaction between particles and the primary and secondary vortices in the lid driven cavity flow. The results show that ellipsoid particles tend to align to the mean flow direction in the near wall region, and the alignment increases with the rise of particle aspect ratio. At a later stage, particle-particle and particle-wall interaction of ellipsoidal particles will also be taken into consideration.

Measurement of bubble parameters in opaque fluids using ultrasound transit time technique

T. Richter (Otto-von-Guericke-University of Magdeburg), T. Wondrak (Helmholtz-Zentrum Dresden-Rossendorf), K. Eckert (TU Dresden), S. Odenbach (Lehrstuhl für Magnetofluiddynamik, Mess- und Automatisierungstechnik, TU Dresden) 17:10

The mapping of the fluid flow and the detection of bubbles is very important for opaque fluids, like liquid metals. In these cases ultrasound techniques can be used. Especially the ultrasound transit time technique (UTTT) possesses advantages for studying the bubble distribution or the contour dynamics.

In order to validate UTTT with standard optical methods, we started with experiments of single Argon bubbles rising in water. The trajectory, the diameter, the terminal velocity and the tilting of the bubbles were measured simultaneously with UTTT and with a high speed camera. The results of both measurements techniques showed a good agreement.

After these calibration measurements first experiments of Ar bubbles rising in GaInSn were performed. In these experiments the bubble behavior was investigated for different

magnitudes of an DC magnetic field in horizontal direction. The parameters of the bubble as well as the velocity of the bubble and of the wake were recorded simultaneously by UTTT and Ultrasound Doppler Velocimetry (UDV), respectively. The results of these measurements were compared with independent measurements using X-ray radiography, which visualized the entire trajectory of the bubble without an applied magnetic field. Without applied magnetic field the bubble showed a zig-zag trajectory with an amplitude larger than 4 mm. The measured bubble diameter alternated during the rise between values of 3.4 mm up to 4.9 mm, which was inflicted by the tilting of the bubble during the zig-zag rise. For an applied magnetic field of 500 mT the bubble trajectory was straightened and the diameters showed regular behavior around 5.3 mm.
Independent x-ray measurements on the same vessel visualized also the zigzag rise and a tilting of the bubble. These results are in good agreement with the UTTT data.
Classification MSC 2010 — 76T10

Numerical investigations of bubbles rising in columns

A. Höffmann (TU Dortmund), P. Ehrhard (TU Dortmund) 17:30

Aeration tanks represent a major energy consumer of municipal wastewater treatment plants. To increase their efficiency, numerical investigations are conducted to capture the hydrodynamics, the mass transfer, and the biochemical reactions in the aeration tank. At first, the hydrodynamics of the bubble rise is computed separately to generate a reliable foundation for the mass-transfer problem.
This work concentrates on numerical investigations of the hydrodynamics in bubble columns with different continuous phases. Herein the bubble-size distribution is assumed to be mono-disperse and the influence of this assumption on the specific mass-transfer area is discussed. To validate the numerical model using experimental results from tomographic measurements, the specific mass-transfer area, gas-volume fraction, and velocity profiles are discussed.

Euler-Lagrange simulations of turbulent two-phase flows with an advanced deterministic bubble coalescence model

F. Hoppe (Helmut-Schmidt-Universität Hamburg, Professur für Strömungsmechanik), M. Breuer (Helmut-Schmidt-Universität Hamburg, Professur für Strömungsmechanik) 17:50

Turbulent bubble-laden flows are encountered in many technical applications especially in the chemical industry, e.g., in bubble column reactors. Besides Euler-Euler simulations predictions based on the Euler-Lagrange approach have become popular and attractive. This modeling concept allows to tackle a variety of physical phenomena based on first principles and is especially suited for dispersed microbubbles. Combining high-fidelity simulation approaches for the continuous phase such as large-eddy simulations with fast and efficient tracking methods for the dispersed phase (see, e.g„ [1, 2, 3]) leads to a valuable prediction tool.
Relying on a deterministic bubble collision model the main topic of the present contribution is an adequate modeling of the coalescence process of microbubbles. For

this purpose, the coalescence model of Jeelani and Hartland [4] has been revisited and improved. It is based on the concept of film drainage describing bubble coalescence by the approach of the bubbles, the trapping of a small amount of liquid between the surfaces of the deforming bubbles and the forcing of the liquid out of the gap leading to a decreasing film thickness. Then either the film thickness reaches a critical minimum leading to film rupture and thus bubble coalescence or the critical thickness is not reached. In this case the bubbles separate from each other restoring their original form. Compared with popular coalescence models such as Prince and Blanch [6] the model has the following benefits: First, instead of a constant contact area a temporally evolving contact surface is taken into account. Second, in case of contaminated bubbles the drainage process is split up into an initially inertia-dominated process followed by a viscous-controlled regime. Third, the determination of the required contact time is done consistently with the film drainage concept.
The model is further improved by assuming a radial pressure gradient which does not contradict the assumption of a radial outflow of the trapped liquid. Additionally, since the transition time between the inertia and viscous-dominated phases cannot be predicted analytically, the present study relies on a numerical solution. However, this procedure would lead to a large CPU-time consumption since the prediction has to be carried out for each individual collision. Thus, an appropriate regression function is set up for a pre-defined range of bubble diameters and relative collision velocities. Consequently, a highly efficient but still fully deterministic bubble collision and coalescence model results applicable for turbulent two-phase flows with a huge number of bubbles.
Two different test cases are taken into account. Since it is difficult to find appropriate experimental data in a controlled environment, as a first setup for which experimental measurements are available, the coalescence of single either clean or contaminated bubbles with a free surface is considered. It is demonstrated that the results are improved compared with more popular but simpler models available in the literature, e.g., Prince and Blanch [6] for clean or Jeffreys and Davis [5] for contaminated bubbles. The second test case considers an ejector type downflow bubble column reactor and the resulting bubble size distribution as a function of the axial location. The corresponding numerical simulations based on the enhanced film drainage model are in progress and will be assessed against the measurements available.

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Application of the Stochastic Field Method to two phase flow

M. Raquet (Karlsruher Institut für Technologie (KIT)), A. Class (Karlsruher Institut für Technologie (KIT)), W. Edelbauer (AVL LIST GmbH) 18:10

The Stochastic Field Method was introduced in the field of combustion and represents a Eulerian Monte-Carlo technique. It was first transfered to the field of multiphase flow in [1] facing a problem in nuclear technology. Within this work it is applied to cavitating flows in the automotive sector. Both phases, the continuous and the dispersed phase, are observed using a Eulerian perspective which fits the architecture of CFD solvers resulting in efficient computations. Instead of solving the behaviour of individual bubbles (as in Lagrangian Particle Methods) variations of volume fractions of the dispersed phase in each computational mesh cell are considered. A stochastic term is introduced into the transport equations for the volume fractions of the dispersed phase via a Wiener process. Thus sampling over several time steps provides the probability density function of volume fraction in each mesh cell. The implementation is carried out by compiling user-functions to a commercial CFD code. A test case representing an injection system in an automotive application is presented. Moreover strategies to implement the effect of coalescence are shown.

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S 11 : Interfacial flows

Friday 09:00 - 11:00 Marienstr. 7, 1st floor, Room 104
Chair: Michael Manhart (TU München)

On transcritical states in viscous flow passing the edge of a horizontal plate

B. Scheichl (Technische Universität Wien), R. Bowles (University College London) 09:00

As proposed by Higuera (*J. Fluid Mech.*, vol. 274, 1994), the shallow-water problem describing a steady planar developed liquid layer under the action of gravity and capillarity and driven by jet impingement over a horizontal plate is to be closed by a specific singular behaviour prescribed at its trailing edge. This singularity can be interpreted

as the classical Burns–Lighthill criterion for vanishing phase speed being met locally. It therefore expresses criticality of developed flow in the usual sense of hampering long waves from making their way upstream. However, this hypothesis must be viewed as unsatisfactory and thus the description of this classical problem as incomplete: it admittedly anticipates the presence of short-sale perturbations anticipating the strong vertical acceleration (by gravity) which the layer undergoes when passing the edge but not their genuine form. Hence, neither is its existence conclusive nor can an alternative expansive singularity, well-known from hypersonic interactive boundary layers, be excluded as long if the flow is scrutinised solely in the long-wave limit. Moreover, it is inevitably associated with a smoothed hydraulic jump and pronounced flow reversal upstream of the edge. It thus does not allow for a gradual transition towards globally supercritical flow howsoever large the jet Froude number is. On the other hand, taking the Reynolds number as arbitrarily large suggests a much more involved asymptotic splitting of the layer without the need to impose that singularity or, equivalently, criticality at the edge. Our completion of the theory puts forward the correct structure of the flow close to the edge which not only renders the shallow-water problem weakly elliptic but also allows the layer pass the edge in a self-consistent manner. We elucidate the circumstances implying Higuera's singularity, how criticality vanishes in the above limits, and how the edge topography affects the local viscous-inviscid interaction.

Investigation of instabilities of a liquid metal/electrolyte interface caused by thermal convection

A. Wiederhold, C. Resagk 09:20

We report about a two-fluid experiment where the behavior of a liquid metal/electrolyte interface is studied. This experiment is a simplified model of a liquid metal battery (LMB) which is a promising device with regard to energy storage and grid stabilization. LMBs generally consist of two liquid metal layers and an electrolyte layer which lies between them. Because hydrodynamic stable interfaces are a key factor for the operation of a LMB, interface deflections caused by thermal convection were investigated. The experiment contains Ga-In-Sn-alloy (Galinstan) as the lower phase and an electrolyte as the upper phase. This two-layer cell is heated from the bottom and cooled from above and represents in principle a Rayleigh-Bénard cell. To measure velocity profiles we apply Ultrasonic Doppler Velocimetry (UDV) for the liquid metal and optical measurement techniques like Particle Image Velocimetry (PIV) for the electrolyte. A Laser triangulation sensor is used to scan the interface and to measure the deflection caused by thermal convection. Measurement results will be presented to give a first estimate whether the interface deflection may impair the operation of a LMB negatively.

Experimental analysis of bell-atomized waterborne paint sprays using optical measurement methods

L. Gödeke (TU Dortmund), P. Ehrhard (TU Dortmund) 10:00

High-speed rotary bell atomizers are used in a wide variety of industrial processes due

to their flexibility and overall performance. The major application fields are spray drying processes and the formation of highly-uniform paint coatings, with the latter being desired in the automotive industry. Accordingly, this process needs to be viable for variable paint flow rates, bell speeds and for different material properties, while maintaining well-defined particle size distributions. The use of appropriate process parameters leads to the desired spray characteristics.
The current work investigates the main influencing process parameters (flowrate, bell speed, bell diameter) and material properties (density, shear viscosity, elongational viscosity, surface tension) for the formation and breakup of the emerging filaments and the resulting spray cone by using Phase-Doppler-Anemometry (PDA) and high-speed imaging. Furthermore the influence of isotropic and anisotropic effect particles on the PDA measurement results has been investigated. The different atomized liquid materials are fully opaque, of non-Newtonian character and differ in their filament breakup due to their rheological behaviour.
The measured local particle size distributions will be area- and flux-averaged and summarized as the global Sauter mean droplet diameter in function of the process and material parameters. A detailed dimensional analysis for this problem that takes into account the elongational viscosity by evaluation of filament breakup-length as a function of the main process parameters is presented. The corresponding dimensionless numbers will be used to describe the physical effects defining the spray formation process by using an Ansatz of powers.

Thin liquid droplet on top of a rotating liquid

K. Boettcher (TU Dortmund), M. Bothe (TU Dortmund) 10:20

In the production of wafers, the spin-coating process is widely used. A liquid droplet is placed on the substrate, wets it, and develops a layer. To accelerate the spreading and to get a thin homogeneous layer, centrifugal forces are created by rotating the substrate. Typically, this is repeated several times. To speed up the process, it is desirable to produce several layers at once. As a first step, the similar but simpler problem of a liquid droplet on top of a second immiscible liquid in a rotating frame is modeled.
If a droplet (liquid lens) is put on a liquid layer, it spreads into the equilibrium of the system which is influenced also by the liquid layer below the droplet. This static equilibrium of a thin liquid lens on the liquid layer surrounded by a passive gas is considered. The system is described by the positions of three free interfaces: lens/layer, lens/gas and layer/gas. The liquids are affected by gravity and centrifugal forces, while at the free interfaces the normal stresses have to be balanced by the curvature pressure drop. After scaling, the lubrication approximation is used to compute analytical solutions for the positions of the free interfaces. As the three phase contact line does not have a fixed position, the line forces are balanced to couple the solutions using a shooting method. If the centrifugal forces are large enough, the liquid lens forms a capillary ridge. For spreading liquids on solids this ridge is known to be the origin of the so-called fingering instability of the contact line. Several liquid fingers start to grow out of the contact line and the areas between the fingers develop unwetted.

In the next step, to extend the model, a stationary system is considered, where the bottom of the layer may be heated or cooled. Here, for both liquids the temperature transport equations have to be taken additionally to the momentum equations into account. As for thin fluid systems, surface effects dominate volume effects only the temperature dependence of the free interface tensions are taken into account. This induces a thermocapillary (Marangoni) shear stress at a free interface. Lubrication approximation is again engaged and three evolution equations are derived, where all conservation laws and all boundary conditions, except for the geometric conditions of the interfaces, are fulfilled. Unfortunately all equations have to be solved numerically. For computation a midpoint trapezoidal method is used, to handle the singularity at the origin.

Experimental investigation of a shear stress driven rotary wave in a cylinder

H. Steinrück (TU Wien) 10:40

The following experimental setup is considered: A vertical cylinder is partially filled with water. The air above the water is set into a rotary motion either by rotating disc or by a rotor. As a consequence, a rotary flow in the water will be induced. It turns out, that above a critical value of the angular speed of the disc or rotor, resp., a rotary wave in the water is excited. Dimensional analysis has revealed two characteristic dimensionless parameters: The base flow in the water is characterized by the Ekman number, while the wave is characterized by the Reynolds number based on the angular wave speed. Stability analysis based on an asymptotic expansion with respect to small Ekman number and large Reynolds number has shown that the base flow is stable if the Ekman number is below a critical value which is proportional to $Re^{-3/4}$. Moreover, it has been shown that the radial shear stress distribution on the free surface is responsible for the instability mechanism. The experiments show that the wave form and the frequency are well described by the potential flow theory. In order to verify the proposed excitation mechanism the surface velocities of the wave will be visualized and compared with the analytical predictions.

S 11 : Interfacial flows

Friday 11:30 - 13:30 Marienstr. 7, 1st floor, Room 104
Chair: Peter Ehrhard (TU Dortmund)

The lift on a small sphere in a linear shear flow near the interface of two immiscible fluids

S. Scheichl (Vienna University of Technology) 11:30

Analytical expressions have been derived which predict, to lowest order, the inertial lift and the lateral migration velocity of a rigid sphere translating and rotating in a linear

shear flow field near the flat interface of two immiscible fluids. This asymptotic analysis is primarily based on the assumption that the two Reynolds numbers defined by the gap width between the interface and the sphere, the shear rate and the translational slip velocity with which the spherical particle moves parallel to the interface are small. Accordingly, the interface lies within the so-called inner region of the sphere's disturbance flow. Furthermore, the radius of the sphere is assumed to be small compared to the gap width. To leading order in this creeping flow regime, the linear Stokes equations are obtained and a symmetry argument can be used to show that the Stokes solution does not predict any lift force. The transverse force experienced by the sphere and its migration velocity are due to the small but finite inertial terms in the Navier-Stokes equations, which can be studied by perturbation techniques.
By applying a Green's function approach and matched asymptotic methods, which also incorporate the effects of the outer Oseen-like flow regime, the three components comprising the lift velocity have been calculated in closed form: the one induced by the shear rate only, the purely slip induced one and the one due to the interaction of the slip velocity with the shear flow field. The thus obtained expressions for the case of two immiscible fluids with arbitrary density and viscosity ratios extend the results that already exist in the literature for other flow configurations, such as an unbounded shear flow field (Saffman 1965) or a wall-bounded one, where the wall lies either within the leading order Stokes region (Cox and Hsu 1977) or in the outer Oseen region (McLaughlin 1991).

Relaxation oscillations of solutal Marangoni convection at droplets and droplet chains

K. Schwarzenberger (TU Dresden), M. Mokbel (TU Dresden), S. Aland (TU Dresden), K. Eckert (TU Dresden) 11:50

Mass transfer of surface-active substances across fluidic interfaces is frequently accompanied by Marangoni instability. Marangoni convection can show a temporal periodicity in the form of relaxation oscillations due to subsequent consumption and regeneration of its driving force. Contrary to the complex behavior of strong surfactants or reactive mass transfer, a simple two-phase-system consisting of paraffin oil and water is employed in our study. Due to mass transfer of isopropanol as a weak surfactant, concentration gradients and, by implication, density gradients are produced in-situ. We have first studied single small droplets, placed in the concentration gradient, by means of a combination of experiments and simulations. The experiments are conducted in a Hele-Shaw experiment in which the doplets are visualized by shadowgraphy. The 2D numerical simulations are based on a diffusive-interface approach and assume a linear concentration and density gradient. We show that the single droplets perform about hundred periods of regular ROs over almost one hour. By analyzing their characteristics, the underlying mechanism can be attributed to the interaction between the mixing by Marangoni convection and the restoring effects of diffusion and buoyant convection on the driving concentration gradients. In the next step, ensembles of droplet comprising droplet pairs as well as linear or circular chains of droplets are investigated. If the spatial distance between the

droplets in within the propagation depth of the relaxation oscillations, we observe an excitation of the relaxation oscillation from one droplet to its neighbor. As a result, neighboring droplets are forced to oscillate with the same frequency. On arranging the droplets in chains, an efficient transmission of the relaxation oscillation can be achieved.

On the Marangoni flow at electrolytically generated hydrogen bubbles

C. Cierpka, D. Baczyzmalski, K. Eckert (TU Dresden), X. Yang 12:10

The application of water electrolysis for energy conversion and long-term storage systems has become a topic of great relevance in view of the worldwide promotion of renewable energy systems. However, one major challenge for the establishment of water electrolysis on an industrial scale is its relatively low efficiency. A significant part of the losses is caused by the formation of hydrogen gas bubbles on the electrode surface. Therefore, considerable research efforts are devoted to gain detailed insights into the bubble nucleation, growth and detachment mechanisms. Local phenomena close to the electrode surface are particularly interesting as the amount of the generated hydrogen gas and its concentration gradients are the largest in this region. Moreover, it was reported that dissolved hydrogen can have a substantial surface activity. Since high concentration gradients of the dissolved hydrogen occur close to the foot of the growing gas bubble, strong gradients of the local surface tension might exist at the gas-liquid interface and could cause significant Marangoni stresses. However, these effects have not been directly observed, mainly due to the experimental difficulties of measuring concentration gradients of dissolved gases at microscopic scales. In this study we aim to gain further insight into this process and demonstrate the existence of these Marangoni stresses by providing detailed measurements of the resulting Marangoni flow near the foot of the bubble. For this purpose, water electrolysis was carried out under potentiostatic conditions in a 1 M H2SO4 solution in a small electrochemical cell. The behavior of a single hydrogen bubble evolving on a microelectrode (100 µm in diameter) was studied by microscopic high speed imaging as well as measurements of the current transient. The flow around the bubble was measure by Particle Tracking Velocimetry (PTV) with additional tracer particles added to the solution. Advanced time-resolved tracking algorithms had to be applied to resolve the fluid motion and its strong velocity gradients in close vicinity of the gas-liquid interface. This flow is obviously the result of the Marangoni stress that is generated by the high concentration gradients of the dissolved hydrogen gas. The results show a good agreement between the production rate of the hydrogen gas and the magnitude of the Marangoni flow. This Marangoni flow might influence the bubble growth by an enhanced mass transfer toward the electrode and affect the coalescence with other bubbles which can be often observed at large electrodes. Furthermore, the Marangoni stresses impose a force on the bubble that could retard the detachment of the bubble from the electrode, which is known to lower the efficiency of the process.

Gas bubbles in round micro-capillaries – PIV measurements and numerical results

P. Lakshmanan (TU Dortmund University), P. Ehrhard (TU Dortmund) 12:30

Process design of multi-phase unit operations on the micro-scale asks for a detailed knowledge of the hydrodynamics and mass transfer. While liquid-liquid plug flow is an often examined phenomenon, gas-liquid flow in small geometries is less common. Although it appears to be a similar problem, in gas-liquid flows surface tension becomes even more dominant and gravity now becomes a non-negligible effect.
The present work focuses on the behaviour of disperse gas bubbles in micro capillaries with a circular cross-section. To examine the velocity field around individual gas bubbles, the micro-PIV technique is applied. To allow for an undistorted view through the glass capillary, a round capillary is manufactured with a planar outer wall, while the refraction index of the liquid is matched to that of the glass capillary to eliminate the refraction from the inner wall of the capillary. Consistent velocity fields can be obtained, even when the matching of the refraction index is not perfect. Experimental results for different modes of operation are compared to numerical simulation and show a good agreement, also to available correlations from literature.

Slow Viscous Flow Near a Superhydrophobic Surface with Trapped Gas Bubbles

A. Ageev (Lomonosov Moscow State University, Institute of Mechanics), I. Golubkina (Lomonosov Moscow State University, Institute of Mechanics), A. Osiptsov (Lomonosov Moscow State University, Institute of Mechanics) 12:50

We study a steady-state Stokes flow of viscous fluid over a periodic striped texture of a superhydrophobic surface (SHS), containing gas bubbles with zero friction. The main aim of the study is to calculate the coefficients of the effective slip length (averaged slip velocities) corresponding to the principal directions of the Bazant-Vinogradova effective slip length tensor [1], which is used in the macroscopic effective slip boundary condition imposed on the SHS. The values of the averaged slip velocities are also used for estimating the drag reduction in microfluidic devices with SH walls. The most common situation is considered, in which the gas bubble surfaces are curved and shifted into the cavities on the SHS. The phase interface is assumed to have the shape of a circle arc, as in the static case. The problem of periodic Stokes flow over one period of the striped texture is split into two problems, corresponding to the flows perpendicular to the stripes and along the stripes. The solution for the flow directed at an arbitrary angle to the stripes is a linear combination of these solutions. Both mathematical problems are solved using the Boundary Element Method (BEM) [2, 3] for the Stokes (flow perpendicular to the stripes) and Poisson (Laplace) (flow along the stripes) equations. An original numerical procedure [4] was developed to solve the boundary integral equations corresponding to the considered problems and to calculate the fluid velocity on/above the phase interface. We performed a parametric numerical study of two kind of flows: (i) a shear-induced flow and (ii) a flow in a narrow channel induced by a given pressure drop. In the limiting

cases (flat phase interface, curved interface pinned at the cavity corners), the results satisfactory coincide with the data known in the literature. On the basis of parametric calculations, it is shown that a shift of the phase interface into the cavity results in a sharp decrease in the effective slip velocity. A possible explanation of the presence of local minima in the averaged slip in the vicinity of the minimal possible radius of the bubble surface is proposed. The method developed and the results obtained can be used for the estimation of the drag reduction in flows near superhydrophobic surfaces. The work received financial support from the Russian Foundation for Basic Research (project No. 16-31-00069).

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3. J.T. Katsikadelis, Boundary Elements: Theory and Applications (Elsevier Science Ltd, 2002)
4. A.I. Ageev and A.N. Osiptsov, “Stokes Flow over a Cavity on a Superhydrophobic Surface Containing a Gas Bubble”, Fluid Dynamics. 50. 748–758 (2015)

S 12: Waves and acoustics

Organizers: Barbara Kaltenbacher (Alpen-Adria-Universität Klagenfurt)
Manfred Kaltenbacher (TU Wien)

S 12 : Waves and acoustics

Tuesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 104
Chair: Barbara Kaltenbacher (Alpen-Adria-Universität Klagen)

Steady two-dimensional transonic flow of BZT fluids

A. Kluwick (TU Wien) 14:00

The dynamic behaviour of compressible fluids depends crucially on the curvature of isentropes in the pressure/specific volume diagram. Most conveniently this curvature is expressed in form of a non-dimensional quantity Γ now commonly referred to as fundamental derivative of gasdynamics, Thompson (1971). Bethe–Zel'dovich–Thompson (BZT) fluids have the distinguishing property that they exhibit embedded regions in the general neighbourhood of the thermodynamic critical point where Γ is negative in contrast to classical gases of low molecular complexity including perfect gases where Γ is strictly positive. The behaviour of steady transonic flows of such fluids is essentially governed by two non-dimensional parameters: Γ and its derivative with respect to the density at constant entropy Λ, Cramer and Fry (1993), Kluwick (1993). The resulting response to external forcing is surprisingly rich in non-classical phenomena such as

rarefaction shocks, sonic shocks, split shocks, etc. and is studied in detail for the canonical problem of two-dimensional flow past compression/expansion ramps.

Thompson, P.A. (1971): *A fundamental derivative in gasdynamics.* Phys. Fluids **14**, 1843–1849.
Cramer, M.S. and Fry, R.N. (1993): *Nozzle flows of dense gases.* Phys. Fluids A **3**, 1246–1259.
Kluwick, A. (1993): *Transonic nozzle flow of dense gases.* J. Fluid Mech. **247**, 661–688.

RANS modeling of sub- and supersonic turbulence – adherence of the characteristic conditions

M. Halder, B. Ghotra, J. Hau, M. Oberlack (TU Darmstadt) 14:20

Essentially all second-moment turbulence models have been developed for incompressible turbulent flows. To extend their applicability to compressible flows, model equations have later been extended towards compressible flows, often in an ad-hoc manner. In order to preserve proper flow physics of propagating waves, we examine whether second-moment turbulence models applied to sub- and supersonic turbulent flows adhere to the characteristic conditions. For supersonic flows this is particularly essential as the real characteristics determine the paths of waves. Only in this case, the wave properties of the regarded flow are represented correctly, i.e. the basic laws of physics are complied.
We compare the characteristics of the original gas-dynamic equations with modelled equations. These are Reynolds- and Favre-averaged gas-dynamic equations together with the transport equations for Reynolds stresses and solenoidal dissipation. From this we present necessary conditions for them to be fulfilled for a proper wave propagation. These conditions depend solely on the parameters of the applied turbulence model and need to be fulfilled in order to correctly represent the underlying wave behaviour. In fact, it is found that not all models admit the correct representation of the characteristics and, hence, wave phenomena are not necessarily correctly captured by all second-moment turbulence model.

Stationary single waves in turbulent open-channel flow

M. Müllner (Institute of Fluid Mechanics and Heat Transfer, TU Wien), W. Schneider (Institute of Fluid Mechanics and Heat Transfer, TU Wien) 14:40

We consider steady two-dimensional turbulent free-surface flow in a channel, with the Froude number Fr of the oncoming flow being slightly above the critical value, i.e. $(2/3)(\mathrm{Fr}-1) = \varepsilon \to 0$. The Reynolds number is assumed to be very large, and the slope of the channel bottom is of the order of ε^2. In this limit, the analysis can be kept free of turbulence modelling. It is known that for a plane bottom with constant roughness, stationary solitary waves in turbulent open-channel flow cannot exist [1]. Thus, various perturbations of the conditions at the channel bottom are considered.
In [1] the roughness of the channel bottom was assumed to vary with the space coordinate to allow small variations in the bottom friction coefficient. The main result was an

extended Korteweg–deVries (eKdV) equation for the non-dimensional, first-order surface elevation. For the steady-state version of this equation an analysis for weak dissipation was pursued. Stationary solitary waves of the classical type, i.e. with strong decay far upstream and far downstream, respectively, were obtained for a piecewise constant bottom roughness with a particular value of a non-dimensional roughness parameter ("eigenvalue"). A stable and an unstable solution were found. The existence of the predicted stable wave was confirmed experimentally [2]. Later, the analysis was generalized to allow roughness parameters that differ from the "eigenvalue". Uniformly valid asymptotic solutions were obtained that describe solitary waves with a shallow downstream tail [3]. Recently, a novel steady-state solution of the eKdV equation was found numerically [4]. It also has the shape of a single wave, but is characterized by a lower crest height.
The present work has two main objectives. First, for the case with varied bottom roughness, the analysis for weak dissipation is used to study the novel kind of single-wave solutions. A uniformly valid solution is obtained that is in good agreement with the numerical solution of the steady-state version of the eKdV equation. Secondly, the boundary conditions at the channel bottom are modified to account for very small variations in the shape of the bottom (e.g. ramps or bumps), while the bottom roughness is assumed constant. An analogy is presented between the bottom shape function and the function that describes the variation in the bottom roughness. As a particular example, a symmetric bump with triangular cross section is considered. The eKdV equation is solved numerically. We show that in this case there are three single stationary waves: The stable and unstable stationary solitary wave, respectively, and the single-wave solution of the new kind.

[1] W. Schneider. Solitary waves in turbulent open-channel flow, JFM 726, 137–159 (2013)

[2] W. Schneider, Y. Yasuda. Stationary solitary waves in turbulent open-channel flow: Analysis and experimental verification, J. Hydraul. Eng. 142(1) (2016)

[3] M. Müllner, W. Schneider. Asymptotic solutions of an extended Korteweg–de Vries equation describing solitary waves with weak or strong downstream decay in turbulent open-channel flow, PAMM 15(1), 491–492 (2015).

[4] R. Jurisits. Degenerate numerical eigensolutions of an extended Korteweg–de Vries equation describing solitary waves in open-channel flow, 11th European Fluid Mechanics Conference (EFMC11), Sevilla (2016)

Hybrid computational aeroacoustics based on compressible flow data at low Mach numbers

S. Schoder (TU Wien), F. Toth (TU Wien), M. Kaltenbacher (TU Wien) 15:00

Lighthill's acoustic analogy transforms the compressible Navier-Stokes equation into an exact inhomogeneous wave equation. When extracting source terms from a compressible

flow simulation, the results already incorporate acoustic wave propagation, corrupting the source term computation. Hence, acoustic analogies based on incompressible flow data are preferred at low Mach numbers. These methods implicitly describe a one-way coupling from flow structures to acoustic waves. However, some practical applications (e.g. a cavity with a lip[1] or resonator like structures) seek for compressible simulation, since acoustic feedback mechanisms excite flow structures. At low Mach numbers we identify the origin of the incompressible part of the velocity field as the incompressible solution of the flow field and the remaining part as a compressible disturbance.
Based on the compressible flow simulation, the acoustic propagation is computed in an extra step. At low Mach numbers, the incompressible flow structures are the main acoustic sources. Therefore, the compressible flow field is separated by the Helmholtz decomposition

$$\mathbf{u} = \mathbf{u}^{\mathrm{ic}} + \mathbf{u}^{\mathrm{c}} = \nabla \times \mathbf{A}^{\mathrm{ic}} + \nabla \phi^{\mathrm{c}} \,, \tag{6.6}$$

where $\mathbf{u}^{\mathrm{ic}}$ represents the solenoidal (incompressible) part and $\mathbf{u}^{\mathrm{c}}$ the irrotational (compressible) part. In this contribution we investigate the two possible computations of $\mathbf{u}^{\mathrm{ic}}$ and the effect on the calculation of the acoustic wave propagation. The scalar potential ϕ^{c} is associated with the compressible part and the property $\nabla \times \mathbf{u}^{\mathrm{c}} = 0$. The vector potential $\mathbf{A}^{\mathrm{ic}}$ describes the incompressible part of the velocity field satisfying $\nabla \cdot \mathbf{u}^{\mathrm{ic}} = 0$. These properties lead to a scalar Poisson problem with the dilatation $\nabla \cdot \mathbf{u}$ as forcing, and to a curl-curl problem with $\nabla \times \mathbf{u}$ as right hand side, respectively. Both methods have been implemented in the finite element software CFS++[2] and are applied to the aeroacoustic benchmark problem of a flow over a cavity with a lip[3].

[1] B. Farkas, G. Paál, Numerical Study on the Flow over a Simplified Vehicle Door Gap - an Old Benchmark Problem Is Revisited. Period. Polytech. Civil Eng., (59)3, 337-346, 2015.

[2] M. Kaltenbacher. Numerical Simulation of Mechatronic Sensors and Actuators: Finite Elements for Computational Multiphysics, 3rd Edition. Springer (2015)

[3] Henderson B., Automobile Noise Involving Feedback- Sound Generation by Low Speed Cavity Flows, In: Third Computational Aerocompressibles(CAA) Workshop on Benchmark Problems, Vol. 1, 2000.

Numerical Prediction of Aerodynamic Noise Generated from an Aircraft in Low Mach number Flight

B. Rasuo (University of Belgrade, Faculty of Mechanical Engineering), V. Jazarevic (University of Belgrade, Faculty of Mechanical Engineering) 15:20

Paper describes numerical prediction of aerodynamic noise generated from an Aircraft. Simulation of turbulent flow is done solving incompressible Navier-Stokes equation, where turbulence is modeled with the orthogonal subgrid scale (OSGS) method with dynamical subscales. Because of comparation, the same simulation is done using the LES (Large Eddy simulation). It is shown how simulation of turbulent flow affects the

prediction of acoustic sources calculated using Lighthill's analogy. Translation from time to frequency domain is done through DFT (Direct Fourier Transform), which give smaller usage of memory. Acoustic sources are used in inhomogeneous Helmholtz equation to simulate pressure wave propagation in the domain. It is shown that OSGS with dynamical subscales give better representation of the spectrum. Overall, better prediction of energy transfer across large and small eddies will give better allocation and presentation of acoustics sources. These sources will change wave propagation of the pressure in acoustic field.

On the sole linear mechanism of acoustic wave generation by vortical perturbations in shear flows

J. Hau (Technische Universität Darmstadt), G. Chagelishvili (Ilia State University), M. Oberlack (Technische Universität Darmstadt) 15:40

We investigate the basics of the linear generation of acoustic waves by vortex modes in homentropic compressible flows with constant shear of velocity, $\mathbf{U}_0 = (Ay, 0, 0)$. The mathematical and physical aspects of the generation are grasped by analyzing the dynamics of single up-shear tilted initially pure vortex spatial Fourier harmonics (SFHs). The key to comprehending the wave generation process is the possibility of splitting the perturbation field of the considered SFH into its vortex/wave parts at the moment of abrupt wave emergence, giving important insights into the linear wave generation mechanism. This is essentially similar in three and two dimensions (3-D and 2-D, respectively), whereas latter dominates the generation process. As the anisotropy of the linear mechanism is also active in 3-D, the conclusion drawn by [3] are confirmed, i.e., the anisotropic linear generation mechanism cannot be captured by any acoustic analogy formulation as introduced by Lighthill [1] due to their topological incompatibility. Further, there exists some freedom in the solution, which enters as a free parameter and has impact on the energy growth of the regarded vortex SFH, eventually leading to the immediate decay of perturbation energy. This parameter is known from the closed-form solution of the incompressible dynamics [2].

[1] M.J. Lighthill *On sound generated aerodynamically – I. General theory* Proc. Roy. Soc. London Ser. A 211, 564-587 (1952).

[2] H.K. Moffatt *Interaction of turbulence with strong wind shear* Nauka Press, Moscow 139-156 (1967).

[3] J.-N. Hau, G. Chagelishvili, G. Khujadze, M. Oberlack, A. Tevzadze *A comparative numerical analysis of linear and nonlinear aerodynamic sound generation by vortex disturbances in homentropic constant shear flows* Phys. Fluids 11, 126101 (2015).

S 12 : Waves and acoustics

Tuesday 16:30 - 18:30 Marienstr. 7, 1st floor, Room 104
Chair: Barbara Kaltenbacher (Alpen-Adria-Universität Klagen)

Adjoint Perturbation Methods for the Investigation of Fixed-Point Iterations Used to Solve Non-Linear Eigenvalue Problems in Thermoacoustics

G. Mensah (TU Berlin), J. Moeck (TU Berlin) 16:30

Thermoacoustic instabilities are a major threat to modern gas turbines. They arise from a self-excited coupling of the unsteady heat release to pressure fluctuations in a combustion system. The acoustics of such a system are commonly modeled in frequency-domain by means of a Helmholtz equation featuring an inhomogeneity accounting for the unsteady heat release. In order to close the problem, this inhomogeneity is often linked to the pressure fluctuation at a reference position by a so-called flame transfer function. Using a discretization method like finite elements, the problem statement then amounts to an eigenvalue problem which is non-linear with respect to its eigenvalue ω:

$$\mathbf{L}(\omega)\hat{p} := \left(\mathbf{K} + \omega\mathbf{C} + \omega^2\mathbf{M} + \mathbf{Q}(\omega)\right)\hat{p} = 0$$

To date the thermoacoustics community uses the fixed-point iteration proposed in [1] to find the mode shapes $\hat{p}$ and corresponding eigenfrequencies ω. This iteration starts with an initial guess for the eigenfrequency which is introduced to the heat release term $\mathbf{Q}(\omega)$. The then quadratic eigenvalue problem is solved for a new eigenvalue. The procedure is repeated until the eigenvalue is not changing anymore. The use of this iteration is especially remarkable, as its convergence properties are unknown. Banach's fixed-point theorem can be utilized to investigate these convergence properties. However, as already outlined in [1] the lack of derivatives of the involved fixed-point operator hinder the use of the theorem. Adjoint perturbations theory fills this gap, because it computes the eigenvalue derivatives of non-linear operator families with respect to certain family parameters. This report discusses how adjoint perturbation theory assesses the contraction properties of the involved fixed-point operator. A notable difference to other acoustic systems and many wave equations in general is the non-self-adjointness of the operator due to the heat release term. The considerations are useful for the choice of starting values for the fixed-point iteration, the automatic setting of a relaxation parameter, and may ultimately be used to tailor new Newton methods tackling the issue.

[1]: Nicoud, F., Benoit, L., Sensiau, C., and Poinsot, T., 2007. "Acoustic modes in combustors with complex impedances and multidimensional active flames". AIAA Journal, 45(2), pp. 426–441.

Anomaly identification in dams using full waveform inversion

M. Alalade (Bauhaus-Universität Weimar), L. Nguyen-Tuan (Bauhaus-Universität Weimar), F. Wuttke, T. Lahmer (Bauhaus-Universität Weimar) 16:50

Drawing inspiration from the successful track record of the application of full waveform inversion (FWI) to subsurface exploration, our proposed method intends to exploit the advantages of FWI in the identification of damages in dams. This is further motivated by the ability of FWI to extract information contained in the complete waveform and its potential of producing high resolution results. Dams are indispensable structures with dominant multiphase-multifield effects which as a result of time induced material deterioration requires frequent health monitoring to prevent structural failure.
The proposed method involves the propagation of mechanical/seismic waves within the dam structure and the mathematical reconstruction of the wave behavior. To ensure stability and also reduce the computational cost inherent in the inversion of waveform, the computational domain is truncated via a perfectly matching layer (PML). The FWI quality is very sensitive to the 'start-up model', thus techniques for a reliable initial model are proposed. Furthermore, optimal source-sensor acquisition set-ups for non-destructive testing in dams are investigated.

An Infinite Mapping Layer for Deep Water Waves

F. Toth (TU Wien), S. Schoder (TU Wien), M. Kaltenbacher (TU Wien) 17:10

When treating open domain problems with the finite element method (FEM) one faces the fundamental problem that the infinite physical domain must be represented by a finite computational domain. Thus, suitable boundary conditions are required at the regions where the domain is truncated. Within the framework of the FEM several methods to handle infinite domains exist, the most prominent probably being the use of so called infinite elements. In this contribution we present a domain mapping method applied to the problem of deep water wave propagation.
We model the water as an incompressible, inviscid fluid. Thus we can describe the wave pressure p in the water domain Ω by

$$\nabla \cdot \nabla p = 0 \quad \text{in} \quad \Omega, \tag{6.7}$$

while the restoring forces due to gravity are incorporated by the linearised free surface boundary condition

$$\frac{\partial^2 p}{\partial t^2} = -g \frac{\partial p}{\partial n} \quad \text{on} \quad \Gamma_f, \tag{6.8}$$

which is valid for non-steep waves. Infinite extension of the water domain in the horizontal direction, i.e. in direction of the water surface, can be handled by a perfectly matched layer formulation [1]. In order to handle the infinite extension in depth direction we introduce an infinite mapping layer at the bottom of the computational domain. In this layer the infinite physical domain is mapped to the finite computational domain using a coordinate transformation.

The method has been implemented in the finite element software CFS++[2]. We explore the performance of different mapping functions and the necessary mapping layer thickness. The method is demonstrated for eigenvalue problems (i.e. the sloshing problem) and harmonic problems (i.e. wave propagation) and validated by comparison to available analytical solutions for deep water waves.

[1] F. Toth, M. Kaltenbacher. Fully coupled linear modelling of incompressible free-surface flow, compressible air and flexible structures. Int. J. Num. Meth. Eng. 107 (2016), 947–969

[2] M. Kaltenbacher. Numerical Simulation of Mechatronic Sensors and Actuators: Finite Elements for Computational Multiphysics, 3rd Edition. Springer (2015)

Linear forced sloshing for a baffled rectangular fuel tank

F. Buck (Daimler AG), E. Fruend (Daimler AG), S. Oexl (Daimler AG), H. Hetzler (University of Kassel) 17:30

Free-surface movements of a liquid in a partially filled tank under external excitation - named sloshing - occur in different applications like spacecrafts [1], liquid cargo ships [2] or tuned liquid dampers [3]. In this contribution fuel tanks of commercial vehicles, which undergo complex three-dimensional excitations, are treated as sloshing effects have to be regarded for an accurate description of the dynamic behavior of the entire commercial vehicle.

For an horizontal excitation of the fuel tank, free-surface modes and corresponding eigenfrequencies can be observed and described by linear potential flow theory (see e.g. [2]) assuming an inviscid and incompressible fluid, irrotational flow and small excitation amplitudes. Vertical excitation, which is very pronounced in trucks due to street unevenness, results in parameter excited vibrations [5]. Using a two-dimensional modal description, the motion of each mode is given by

$$\ddot{\beta}_m(t) + 2\xi_m\omega_m\dot{\beta}_m(t) + \omega_m^2\left(1 + \frac{\ddot{z}_0(t)}{g}\right)\beta_m(t) = -\frac{\lambda_{1m}}{\mu_m}\ddot{x}_0(t), m \in \mathbb{N}$$

in the case of linear viscous damping with eigenmode $\varphi_m(x,z)$, eigenfrequency ω_m and free-surface elevation $\zeta(x,t) = \sum_{m=1}^{\infty}\beta_m(t)\varphi_m(x,0)$. $\ddot{x}_0(t)$ and $\ddot{z}_0(t)$ denote the horizontal and vertical excitation, respectively. The hydrodynamic coefficients $\lambda_{1m} = \rho\int_{\partial V_f}\varphi_m(x,0)x\mathrm{d}x$ and $\mu_m = \frac{\rho}{\kappa_m}\int_{\partial V_f}\varphi_m(x,0)^2\mathrm{d}x$ are integrals over the fluid surface ∂V_f and the resulting horizontal sloshing force can be calculated by

$$F_x = -m_{\mathrm{Fluid}}\ddot{x}_0(t) - \sum_{m=1}^{\infty}\ddot{\beta}_m(t)\lambda_{1m}.$$

Eigenfrequencies and eigenmodes as well as corresponding damping values have to be determined to predict the free-surface shape and occurring sloshing forces. Fuel tanks of

commercial vehicles have an approximately rectangular shape and are typically designed with perforated plates as baffles. Therefore, the numerical procedure given by Faltinsen [5] for a tank with a centrally mounted screen is applied and extended to calculate the eigenfrequencies and eigenmodes for tanks subdivided by baffles at different positions. Beside the inner fluid damping and the damping due to viscous boundary layers, the sloshing amplitudes are mainly reduced by the pressure drop at the inserted baffles, which can be incorporated in the given modal description [6].
Resulting eigenfrequencies, mode shapes and horizontal forces are investigated and validated with experimental results. Furthermore, stability regions are determined experimentally and the effect of damping due to integrated damping devices on the Ince-Strutt stability diagram is examined.

[1] H. N. Abramson. The dynamic behavior of liquids in moving containers. NASA SP-106. NASA Special Publication 106 (1966).

[2] O. M. Faltinsen, A. N. Timokha. Sloshing. Cambridge University Press (2009).

[3] M. J. Tait, A. A. El Damatty, N. Isyumov, M. R. Siddique. Numerical flow models to simulate tuned liquid dampers (TLD) with slat screens. Journal of Fluids and Structures 20 (2005), 1007–1023.

[4] R. A. Ibrahim. Liquid sloshing dynamics: theory and applications. Cambridge University Press (2005).

[5] O. M. Faltinsen, A. N. Timokha. Natural sloshing frequencies and modes in a rectangular tank with a slat-type screen. Journal of Sound and Vibration 330 (2011), 1490–1503.

[6] O. M. Faltinsen, R. Firoozkoohi, A. N. Timokha. Steady-state liquid sloshing in a rectangular tank with a slat-type screen in the middle: Quasilinear modal analysis and experiments. Physics of Fluids 23 (2011), 042101.

Generation of surface waves through friction: FEM investigation

M. Graf (Hochschule Emden/Leer) 17:50

Sliding friction between two bodies can generate elastic vibration. There are many mechanisms known that cause these vibration, e.g. mode coupling or a velocity-dependent falling coefficient of friction. This study investigates friction induced waves similar to the Rayleigh wave. It uses a finite-element model comprising an elastic body sliding against a rigid surface with constant coefficient of friction. In some cases the simulation shows travelling surface waves, which depend on the structure of the sliding surface. It can be shown that the surface structure and its inertia are the cause for elastic waves in the contact region. Furthermore the excitation mechanism of these travelling waves is analyzed.

Optimization of 3D-Waveguides using Finite Elements and Transformation Optics

P. Kraft (KIT) 18:10

Solving complete 3D-Maxwell problems using Finite Elements is a very computationally expensive operation. However, for the evaluation of more simplified models it is a required tool. We present an approach based on Transformation Optics to reduce the computational cost of such simulations. On one hand the large condition number of system matrices resulting from the application of Nédélec elements to Maxwell's equations usually prevent the usage of iterative solvers. On the other hand the high number of required degrees of freedom to approximate the oscillatory nature of the solution discourage the usage of direct solvers. For very few degrees of freedom of the shape of the waveguide we have shown in a previous publication that on the one hand solving the forward problem (simulation of the signal propagation based on the finite element method) numerically is feasible and on the other hand even inverse problems (optimization of the shape) can be dealt with. Since solving forward problems in this case is extremely costly and a finite-difference-type method for the approximation of the shape gradient scales linearly in the number of shape parameters, this method cannot be applied to scenarios, in which a high number of shape parameters is required. To circumvent this problem, we do experiments on an adjoint-based optimization scheme which also enables us to perform line searches for a high number of parameters (rather then an approximation of the shape gradient) whilst causing low numerical cost. The current state of this research will be the topic of this talk.

S 12 : Waves and acoustics

Wednesday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 104
Chair: Florian Toth (TU Wien)

Elastic wave radiation and scattering in heterogeneous soil using the scaled boundary finite element method

C. Birk (Universität Duisburg-Essen), H. Gravenkamp (Universität Duisburg-Essen), M. Bazyar (Yasouj University) 14:00

The numerical simulation of radiation and scattering of elastic waves in the soil is required when predicting the effect of ground motion or when modelling the propagation of vibrations induced by trains in tunnels, for example. Here, two major challenges exist. Firstly, the soil typically is of very large extent and can be idealized as unbounded. Thus, radiation damping must be accounted for. Secondly, efficient modelling techniques are required to handle potentially large near field domains. Seismic analyses may require the resolution of geometrical features at very different scales. Moreover, specific mesh requirements exist for wave propagation analyses depending on material properties and frequency content.

In this contribution, the above challenges are addressed by the scaled boundary finite element method (SBFEM) - a semi-analytical method which excels in modelling dynamic problems in unbounded domains. An approach is presented, which is based on splitting the problem domain into a regular far field region and an irregular, potentially highly heterogeneous near field region. Using the SBFEM, a unit-impulse-response-based representation of the far field is obtained, where radiation damping is modelled rigorously. The near field region is modelled using a quadtree mesh, which allows for rapid transitions in mesh resolution at material boundaries and geometrical discontinuities. If information regarding the material distribution in the near field region is available in digital form, a corresponding quadtree mesh can be created automatically using image-based techniques. The scaled boundary finite element method facilitates wave propagation analyses on such structured meshes without the need of additional treatment of hanging nodes. Here, high-order elements can be incorporated to relax the requirements with respect to the number of nodes per wavelength. Individual element orders can be chosen automatically based on material properties and size of individual quadtree cells. The combined quadtree-unit-impulse-response-based approach for wave propagation in heterogeneous soil domains is illustrated studying several radiation and scattering phenomena.

Wave Propagation in a beam with random material properties

E. Zimmermann (Helmut Schmidt Universität - Universität der Bundeswehr Hamburg), R. Lammering (Helmut Schmidt Universität - Universität der Bundeswehr Hamburg) 14:20

Modern composite materials, e.g. carbon fiber reinforced plastics, exhibit a complex microstructure due to their fabrication process. The latter, usually omitted in mechanical models through the homogenization of elastic properties, has a strong influence on the propagation of ultrasonic guided waves [1], [2]. Though it is possible to model the wave phenomena deterministically, taking into account a realistic distribution of fibers and polymer matrix, it is essential to develop an improved model for the finite element analysis (FEM), which considers the stochastic properties in a more general way. In the current work, an approach for the simulation of waves in structures with random material properties is presented. For the numerical computations with the FEM a discretization of these properties is necessary. For this purpose, the material properties are expanded in a Fourier-type series with known covariance, also called Karhunen-Loève Expansion (KLE). From this system with a random input field one obtains a solution which is also a random field but with unknown covariance. To handle this problem an alternative expansion is needed. It is assumed that the random variables are orthonormal Gaussian and therefore the Polynomial Chaos (PC) is used to expand the solution. The combination of the KLE with the PC results in the well know Spectral Stochastic Finite Element Method [3]. In a first study step, an isotropic beam model is considered. It is assumed that the Young's modulus is the realization of a Gaussian random field over the spatial domain occupied by the beam. Numerical investigations on the excited and propagating guided waves are presented.

[1] M. N. Neumann, B. Hennings, R. Lammering: Quasi-continuous mode conversion of Lamb waves in CFRP plates due to inhomogeneity on micro and meso scale. 7th European Workshop on Structural Health Monitoring, Nantes, France, 2014
[2] B. Hennings, R. Lammering: Material modeling for the simulation of quasi-continuous mode conversion during Lamb wave propagation in CFRP-Layers. Composite Structures, 150, 2016
[3] Ghanem R. G., Spanos P.D.: Stochastic Finite Element: A Spectral Approach. Springer-Verlag, 1991

Lamb wave resonance transmission through a system of deep notches in a plate-like waveguide

E. Glushkov (Kuban State University), N. Glushkova (Kuban State University), A. Eremin (Kuban State University), R. Lammering (Helmut-Schmidt-Universität) 14:40

Interaction of elastic guided waves with a system of sharp obstacles is expected to result in extended frequency ranges of wave shielding (gap bands). However, not infrequently a resonance wave passing at certain frequencies within those gap bands is also observed [1-3]. Such a phenomenon, originating physically from localized modes concentrated in the damaged area, is mathematically conditioned by nearly real complex-valued spectral points (eigenfrequencies) of the corresponding diffraction boundary value problem, which takes into account all the obstacles simultaneously [1,2].
In this talk the results of theoretical and experimental investigation into resonance phenomena occurring in the course of guided wave propagation in a metallic plate with a finite system of regular prolonged deep notches are presented and discussed. Numerical evaluation of diffraction resonance frequencies is based on the plane-strain assumption and relies on semi-analytical models of various complexity ranging from first-order plate theories to the general equations of linear elastodynamics. Experimental investigations are carried out for aluminium specimens with machined surface grooves. The incident waves are excited by surface mounted piezoelectric wafer active sensors while a contactless laser Doppler vibrometry is utilized for the wave propagation sensing and visualization.
Simulation and experimental results have confirmed the expected intensification of wave blocking by a system of notches comparing to the case of a single defect. And the resonance transmission at the predicted frequencies within these forming gap bands is also observed. The number of the resonance transmission peaks inside the gap bands is proportional to the number of obstacles. Noticeable motion localization in the waveguide area between the notches at these frequencies is visualized with surface B-scans. Their patterns coincide with the theoretical predictions obtained on the basis of semi-analytical computer models for the notched infinite plate as well as with the FEM obtained eigenmodes of its finite part containing all the obstacles.
1. E. Glushkov, N. Glushkova, M. Golub, A. Eremin, Resonance blocking and passing effects in two-dimensional elastic waveguides with obstacles, J. Acoust. Soc. Am. 130 (1), 113–121 (2011) 2. E. Glushkov, N. Glushkova, J. Wauer, Wave propagation in an

elastically supported string with point-wise defects: gap-band and pass-band effects, ZAMM - Z. Angew. Math. Mech. 91(1), 4-22 (2011) 3. R.P. Moiseyenko, Y. Pennec, R. Marchal, B. Bonello, B. Djafari-Rouhani, Broadband attenuation of Lamb waves through a periodic array of thin rectangular junctions, Physical Review B 90, 134307 (2014)

Optimization of the piston geometry to generate a desired stress wave shape

J. Burgert 15:00

In the long history of rock drilling, fundamental mechanisms contributing to the effective drilling process are still unknown. To produce maximal tool penetration for each hit rules should be derived which specify the dimensioning of the piston and drill rod. Recent investigations that cover the issue of optimization are revealing that the efficiency of the drilling process strongly depends on the shape of the longitudinal wave transmitted through the drill rod to the drill bit. A well-known fact is that the cross-sectional profile of the piston is shaping the stress wave profile. Therefore, one approach is to adjust the geometrical form of the impacting piston for an optimized shape of the stress wave from which a maximal penetration follows. The challenge in modelling is the collision between the piston and the rod which leads to a sudden velocity jump at the contact zone. Thus, the non-smooth problem makes the problem difficult to calculate with commercial FE-programs. For an analytical solution, the piston geometry is modelled with piecewise constant cross sections. On a constant segment, the solution of the wave problem is known by the d'Alembert solution. At each change of the cross section the incoming wave is partly reflected and partly transmitted which is considered by transition conditions. This results in a multitude of transmissions and reflections that are all contributing to the final shape of the stress in the drill rod. By using a large number of segments, any piston shape can be approximated. In this contribution, typical piston geometries are investigated where the stress over time is presented along with the associated energy transfer between the piston and the drill rod. Finally, the results of the optimization are discussed

Non-equilibrium Magnetosonic Wave Motion

W. Ellermeier (TU Darmstadt) 15:20

In ideal compressible hydrodynamics there is an isomorphism between spatially one-dimensional unsteady and two-dimensional steady supersonic flow called piston analogy. This note shows that this is also true for non-equilibrium magnetosonic flow under alignment of undisturbed flow and magnetic field in case of steady flow. An example for two generic problems, i.e. the signal problem of radiation into a half space and steady flow along a kinked wall bounding a half space, is given.

S 13: Flow control

Organizers: Holger Foysi (Lehrstuhl für Strömungsmechanik)
Nicolas Gauger

S 13 : Flow control

Friday 09:00 - 11:00 Marienstr. 7, 1st floor, Room 106

On the Convergence of Approximations to Riccati-based Boundary-feedback Stabilization of Laminar Flows

J. Heiland (Max Planck Institute for Dynamics of Complex Technical Systems), P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems) 09:00

Riccati-based feedback is commonly applied for the stabilization of incompressible Navier–Stokes equations in theory ([Raymond(2006)]) and in simulations ([Benner and Heiland(2015)]). Nonetheless, only few attempts were made to show the convergence of numerically computed feedback gains to the feedback defined by the actual model.
There are two major difficulties in the numerical analysis of finite element approximations to the Riccati-based feedback controller for incompressible Navier-Stokes equations. Firstly, the standard approach of mixed finite element only defines an external approximation to the space of divergence free functions so that the standard Galerkin theory does not readily apply. Secondly, boundary control problems typically lead to unbounded input operators.
In this talk, we investigate how standard finite-dimensional define stable and convergent *external* approximations to solutions of incompressible Navier–Stokes equations and extend known results on convergence of Riccati solutions ([Ito(1987)]) in standard Galerkin schemes. Also, we discuss how the necessary uniform boundedness of the discrete input operators can be achieved by a relaxation of the Dirichlet boundary conditions.

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[Ito(1987)] K. Ito. Strong convergence and convergence rates of approximationg solutions for algebraic Riccati equations in Hilbert spaces. In *Distributed parameter systems, Proc. 3rd Int. Conf., Vorau/Austria*, pages 153–166, 1987.

Derivative Instabilities in Active Flow Control with Navier-Stokes Equations

E. Özkaya (TU Kaiserslautern), N. Gauger (TU Kaiserslautern), D. Marinc (Uni Siegen), H. Foysi (Uni Siegen) 09:20

Gradient based numerical optimization is an efficient way to determine the optimal values of control parameters in active flow control problems, especially if the dimension of the control vector is very large. The instabilities of the control sensitivities, however, poses a potential problem since the sensitivity results can be too large when the objective function is a quantity that is evaluated over a long time horizon. This failure is caused either by numerical instabilities that might occur as a result of poor numerical treatment or physical instabilities that are inherently present in the flow. In the present talk, we investigate the effect of physical instabilities on the control sensitivities on a round jet configuration with Re = 10,000, in which the flow is resolved with a LES simulation. The control sensitivities are obtained from a tangent-linear LES solver, which has been generated by applying Algorithmic Differentiation (AD) techniques to the primal flow solver. Since exact derivatives are propagated in forward-in-time using AD techniques, the sensitivity results do not suffer from the cancellation errors that typically occur in finite difference approximations.

A new averaging approach to numerically calculate the adjoint solution of chaotic systems as the Lorenz-attractor or the Navier-Stokes-equations

S. Knechtel (TU Berlin), J. Sesterhenn (TU Berlin) 09:40

In the last decades the adjoint method has become a wildly used and researched method in numerical fluid dynamics, e.g. for design optimization or noise reduction problems. Typically a partial differential equation is solved using a time-stepping method in positive time direction. With this solution the linear adjoint operator is built and solved using the same time-stepping method backwards in time.
This typical approach fails when used on difference equations that have unstable fixed points according to linear stability theory. In this case the backward adjoint calculation is unstable and the solution diverges, as with chaotic systems like the Lorenz-attractor [1] or the turbulent Navier-Stokes-equations.
When calculating the sensitivities of averaged quantities this presents a big problem: In practice artificial damping is used or only a very short time frame is considered, which leads to biased sensitivities and subsequently to only moderate optimization.
A recently developed approach makes it possible to compute sensitivities of ensemble-averaged solutions of chaotic systems via the adjoint method [2]. Unfortunately, this procedure is not yet applicable on big systems with today's computing power. This is because, after conducting several computations forward in time to get the ensemble-averaged solution, a linear equation system has to be solved that has the size of all spatial and temporal degrees of freedom.
We present, using the example of the Lorenz-attractor, a new approach for systems that possess a stationary time averaged solution. The procedure is as follows: After computing the forward solution, an averaged, stationary adjoint operator is constructed using a heuristic ansatz for the closure problem. The sensitivities can now be calculated

either by directly solving the resulting linear equation system or by devising a stable, but stiff partial differential equation, whose stationary solution can be obtained with implicit pseudo-time-stepping methods.
In contrast to the above-mentioned approach, only one forward solution has to be computed and, instead of storing the state variables at all times, only the time averaged quantities have to be saved. The resulting linear equation system is by the factor of the temporal degrees of freedom smaller and for most problems accessible by today's parallel linear equation solvers. For very big systems implicit pseudo-time-stepping can be employed, which is a commonly used method in computational fluid dynamics.
The applicability of our method to the Navier-Stokes-equations is subsequently discussed using the example of a two-dimensional turbulent free shear flow. We compare different closure ansatzes for the time averaged adjoint operator and discuss the computation of sensitivities of both time averaged quantities and their variances.

[1] D.J. Lea, M.R. Allen and T.W.N. Haine: *Sensitivity analysis of the climate of a chaotic system.* Tellus 52 (2000), 523-532.

[2] Q. Wang: *Forward and Adjoint Sensitivity Computation of Chaotic Dynamical Systems.* Journal of Computational Physics 235 (2013), 1-13.

The shifted proper orthogonal decomposition (sPOD): On the boundary treatment for a mode decomposition for multiple transport phenomena

J. Reiss (TU Berlin), P. Schulze (TU Berlin), V. Mehrmann (TU Berlin) 10:00

Reduced-order models can reduce the effort of optimization, control, and parameter studies of complex physical systems. The effort is reduced only if the system can be described by a low dimensional model, i.e. if few modes are sufficient to describe the full system. However, transport-dominated phenomena still provide a challenge since usually common model reduction approaches yield many modes, leading to a high dimensional model.
In this talk, we consider a recently developed model reduction technique, which extends the proper orthogonal decomposition (POD). The snapshot matrix is decomposed into multiple co-moving frames separating the dynamics into the different moving modes, reducing the number of modes in many problems.
Here, we discuss strategies for the boundary treatment, which is important in many practical applications. The full method is purely data based.

Experimental investigation of the effect of aircraft trailing vortices on roofs

A. Uhl (RWTH Aachen University), S. Braun (Deutsches Zentrum für Luft- und Raumfahrt e. V.), S. Hille (RWTH Aachen University), R. Hörnschemeyer (RWTH Aachen University), E. Stumpf (RWTH Aachen University) 10:20

Roofs of buildings in the vicinity of airports can be damaged by trailing vortices of aircraft during take-off and landing. In the past years numerous cases have been documented in which roof tiles were damaged over a large area. In literature, the loads occurring onto the roof are described as a result of the suction force produced by the tangential velocity of the trailing vortices. However, it seems that these forces are not able to cause such roof damages.
Experimental investigations have been conducted in the ILR water towing tank using a generic high-lift wing crossing a house model made of acrylic glass. The facility consists of a 9 m long tank with a cross section of 1.5 m $\times$ 1 m. Copper strips were installed on the model's saddle roof as well as on the high-lift model for flow-visualization by means of hydrogen bubbles. The experiment was recorded using a camera which was placed perpendicular to the trailing vortex axis.
The results presented here show that shortly before the vortex comes into contact with the roof, a bending of the vortex axis followed by a complete breaking up of the trailing vortex can be observed. The part of the vortex facing the wing model is bended in a way that its vortex core comes into contact with the roof surface. As a result of this contact, the suction force is significantly greater due to very low pressure in the vortex center. Afterwards, this vortex moves downwards on the roof similar to a tornado, which is consistent with already documented damages on real roofs.

Drag reduction of spanwise transversal traveling surface waves with stepwise amplitude increase

P. Meysonnat (Institute of Aerodynamics, RWTH Aachen University), 10:40
M. Albers (Institute of Aerodynamics, RWTH Aachen University), W. Schröder (Institute of Aerodynamics, RWTH Aachen University)

Drag reduction in turbulent boundary layer flows is one of the key methods for substantial energy savings in aircraft design. Large parts of the flow over the wing of modern aircraft is turbulent, thus even net energy savings of a few percent can lead to high cost savings. Therefore, numerous techniques have been investigated in the past for passive and active turbulent flow control. Among the passive techniques are riblet surfaces, which can decrease drag by up to 10 percent for a riblet height of $A^+ = 15 - 20$ in inner units [1]. In active flow control, it was shown that spanwise oscillating walls can decrease the friction drag by up to 50 percent in turbulent channel flows [2]. Another promising approach is the spanwise transversal traveling surface waves which impose a secondary flow field in the spanwise direction. Studies in channel flows have shown drag reductions of 30 percent [3], while the effect in turbulent boundary layers is in the range of 10 percent [4].
One aspect of the spanwise traveling wave technique, that has not been under investigation yet, is the response time of the flow to sudden changes of the wave input parameters. The time scales, necessary for the turbulent flow to adapt to a changed amplitude or wave speed, are interesting in the context of future closed loop control strategies. Therefore, in this study a turbulent boundary layer flow is subject to a spanwise traveling wave actuation with increasing amplitude. The immediate effect of rapid amplitude changes

and the convergence to a new steady state are the key factors in this investigation. The numerical simulations are performed using a zonal RANS/LES approach with a high near wall resolution to accurately capture the bulk of the turbulent fluctuations in the near wall region. For the LES, no explicit turbulence model is used but the monotonically integrated LES approach is taken. The physical domain is kept small due to the high Reynolds number and a turbulent flow field is generated at the inflow by the synthetic turbulence generation method and superposed to a mean velocity profile. The sinusoidal spanwise surface wave is prescribed by the analytical expression

$$y^+|_{\mathrm{wall}}(z^+, t^+) = A^+ \cos\left(\frac{2\pi}{\lambda^+} z^+ - \frac{2\pi}{T^+} t^+\right) \tag{6.9}$$

at the wall, with z^+ being the spanwise coordinate, t^+ the time, A^+ the amplitude, λ^+ the wavelength, and T^+ the period of the wave in inner coordinates, i.e., normalized by the friction velocity $u_{\tau,i}$ at the inlet and the kinematic viscosity ν. All investigated configurations possess a wavelength of $\lambda^+ = 500$, a period of $T^+ = 80$ in inner units at a Reynolds number $Re_\theta = 2000$ and a Mach number of $M = 0.2$. The amplitude is rapidly increased from $A^+ = 0$ to $A^+ = 10$, $A^+ = 30$, and $A^+ = 50$ during the computation and a smooth transition from the non-actuated part to the actuated part of the plate is used. The simulation shows an increase of the integrated wall-shear stress of 2 percent for $A^+ = 10$ and drag reduction rates of 7 percent for $A^+ = 30$ and 10 percent for $A^+ = 50$. A new steady state of the flow, subject to the altered actuation, is reached within 150 non-dimensional time units. Further results of the numerical investigation will be presented at the conference.

[1] Bechert DW, Bruse M, Hage W, and Van der Hoeven JG Th, Hoppe G. Experiments on drag-reducing surfaces and their optimization with an adjustable geometry. Journal of fluid mechanics 1997;338:59–87.
[2] Quadrio M. Drag reduction in turbulent boundary layers by in-plane wall motion. Philosophical Transactions of the Royal Society of London A: Mathematical, Physical and Engineering Sciences 2011;1940:1428–1442.
[3] Zhao H, Wu JZ, and Luo JS. Turbulent drag reduction by traveling wave of flexible wall. Fluid Dynamics Research 2004;34(3):175-198
[4] Koh SR, Meysonnat P, Statnikov V, Meinke M, Schröder W. Dependence of turbulent wall-shear stress on the amplitude of spanwise transversal surface waves. Computers & Fluids 2015;119:261–275.

S 13 : Flow control

Friday 11:30 - 13:30 Marienstr. 7, 1st floor, Room 106

Numerical investigation of vortex roll-up processes using different wingtip shapes

A. Uhl (RWTH-Aachen University), S. Dufhaus (RWTH-Aachen University), R. Hörnschemeyer (RWTH-Aachen University), E. Stumpf (RWTH-Aachen University) 11:30

As a consequence of lift generating surfaces, wingtip vortices are an unavoidable result of flying aircraft. They pose a potential risk for following aircraft due to strong coherent flow structures. Stability characteristics of these vortices are related to the axial velocity component within the vortex core. It is known that, in the near field, the axial velocity component is largely affected by the tip shape.
Vortex roll-up processes of three different generic wingtip shapes at a Reynolds Number of $\mathrm{Re} = 1,200,000$ are investigated using the DLR-TAU flow solver combined with the SSG/LRR-ω Reynolds Stress Model. The spatial discretization of the simulation is provided by an unstructured mesh using the CENTAUR mesh generator.
It will be shown that, depending on the angle of attack, a rectangular tip leads to an axial velocity excess while a rounding of a tip leads to an axial velocity deficit in the vortex core. This axial velocity component seems to be related to the vortex topology during the roll-up process. While the roll-up process of a rectangular tip is characterized by a single discrete vortex, multiple vortices are created at elliptically rounded tips. These multiple vortices start to merge at the trailing edge causing axial velocity components that are lower than the freestream velocity.

Modal analysis of wing tip vortices by means of Proper Orthogonal Decomposition

S. Dufhaus (RWTH-Aachen University), S. Brautmeier (RWTH-Aachen University), A. Uhl (RWTH-Aachen University), R. Hörnschemeyer (RWTH-Aachen University), E. Stumpf (RWTH-Aachen University) 11:50

This paper discusses the influence of different wing tip geometries on relative high energetic eigenmodes of wing tip vortices. Based on the results found by Fabre et al., these eigenmodes are a key factor for the stability analysis.
Experiments have been performed at the circulating water tunnel of the Institute of Aerospace Systems (ILR) Aachen. The freestream velocity was adjusted so that a constant Reynolds number of $\mathrm{Re} = 1.45$ Mio. was achieved. The chord length of the investigated models is $c = 400$ mm and the aspect ratio is $\mathrm{AR} = 1.5$.
The measurement technique of stereo particle image velocimetry (S-PIV) was used to determine the velocity components in all three dimensions, u, v and w, whereas u is directed in flow direction (x axis of a right-handed coordinate system). The measurement plane was fixed at $x/c = 0.35$ behind the trailing edge perpendicular to the freestream

velocity.
For image acquisition and data reduction the Lavision Software Davis 8.3. is used. After vector processing a POD analysis to detect the most energetic eigenmodes in the vortex core was performed. In comparison to the results found by Fabre et al., some special kinds of modes have been detected. In literature these modes are related to different instabilities. For example, the wing tip with an elliptic rounding shows a spiral-like mode (m = 1) leading to a displacement wave. This can cause long-wave cooperative instability. A wing tip with a smaller semi axis of an ellipse rounding shows a double helical wave (m = 2). This mode can lead to a damping of further disruptions.
Further research is needed to check whether the instability mechanism far downstream can be predicted by the modal analysis. Furthermore a sensitivity study on mode detection should be done.

S 14: Applied analysis

Organizers: Maria Neuss-Radu (FAU Erlangen-Nürnberg)
Marita Thomas (Weierstrass Institute for Applied Analysis and Stochastics)

S 14 : Applied analysis

Tuesday 14:00 - 16:00 Weimar hall, Large hall

Sharp Interface Limit for a Stokes/Allen-Cahn System

H. Abels (Universität Regensburg), Y. Liu 14:00

We consider a simplified diffuse interface model for a two-phase flow of two macroscopically immiscible fluids with phase transition, which leads to a coupled Stokes/Allen-Cahn system. For this model we discuss the singular limit when a parameter $\epsilon > 0$ that is proportional to the thickness of the diffuse interface tends to zero. For sufficiently small times we prove convergence of the solutions of the Stokes/Allen-Cahn system to solutions of a sharp interface model, where the interface evolution is given by the mean curvature equation with an additional convection term coupled to a two-phase Stokes system with an additional contribution to the stress tensor, which describes the capillary stress.

Diffuse interface models in Biology

E. Rocca (University of Pavia) 14:20

We consider a recently proposed diffuse interface model for tumor growth where sharp interfaces are replaced by narrow transition layers arising due to adhesive forces among the cell species. Hence, a continuum thermodynamically consistent model is introduced. The resulting PDE system couples four different types of equations: a Cahn-Hilliard

type equation for the tumor cells (which include proliferating and dead cells), a Darcy law for the tissue velocity field, whose divergence may be different from 0 and depend on the other variables, a transport equation for the proliferating (viable) tumor cells, and a quasi-static reaction diffusion equation for the nutrient concentration. We establish existence of weak solutions for the PDE system coupled with suitable initial and boundary conditions. In particular, the proliferation function at the boundary is supposed to be nonnegative on the set where the velocity u satisfies $u \cdot n > 0$, where n is the outer normal to the boundary of the domain.
Joint work with M. Dai, E. Feireisl, G. Schimperna, M. Schonbek

A coupled bulk-surface model for lipid raft formation in cell membranes

A. Rätz (TU Dortmund) 14:40

In this talk, we investigate a model for lipid raft formation and dynamics in biological membranes. The model describes the lipid composition of the membrane and an interaction with cholesterol. To account for cholesterol exchange between cytosol and cell membrane we couple a bulk-diffusion to a surface PDE on the membrane. The latter describes a relaxation dynamics for an energy taking lipid-phase separation and lipid-cholesterol interaction energy into account. It takes the form of an (extended) Cahn–Hilliard equation. We choose diffuse-interface methods, in order to simulate the coupled bulk-surface system. Moreover, we consider the limit of infinitely fast bulk diffusion, where one obtains a reduced non-local surface PDE model. This reduced model is numerically treated by surface finite elements and its stationary points are analyzed.
AMS Subject Classification: 35K51, 35K71, 35Q92, 92C37, 35R37

Analysis of recent Nernst-Planck-Poisson-Navier-Stokes systems of electrolytes

P. Druet 15:00

Recently Dreyer, Guhlke and Müller proposed a new non-equilibrium model for liquid electrolytes in accordance with the universal balance laws for mass and momentum, and with the second principle of thermodynamics. This model decisively improves the classical Nernst-Planck theory of electrolytes in several respects. In particular, pressure contributions and charge accumulation near to boundary layers can be accounted for. Moreover, the thermodynamic approach leads to new structures concerning the diffusion fluxes and the highly non-linear rates for the chemical reactions. In the talk we will shortly present the model and an existence result for global-in-time weak solutions.

Compressible multicomponent porous media flow with Maxwell-Stefan diffusion

L. Ostrowski (Institute of Applied Analysis and Numerical Simulation, University of Stuttgart), C. Rohde (Institute of Applied Analysis and Numerical Simulation, University of Stuttgart) 15:20

The dynamics of multicomponent flows in porous media show situations which demand,

in order to be described properly in a mathematical model, a more complex diffusion law than the classical Fickian one.
For this purpose we introduce a macroscale model which makes use of Maxwell–Stefan diffusion terms. For $n \in \mathbb{N}$ constituents of the fluid mixture and constant temperature $T_* > 0$ the governing equations read as

$$\begin{aligned} \partial_t \rho_i + \operatorname{div}(\mathbf{m}_i) &= 0, \\ \partial_t(\mathbf{m}_i) + \operatorname{div}\left(\frac{\mathbf{m}_i \otimes \mathbf{m}_i}{\rho_i} + p_i(\rho_i)\boldsymbol{I}\right) &= -M_i \mathbf{m}_i - T_* \sum_{j=1}^{n} \lambda_{ij}(\rho_j \mathbf{m}_i - \rho_i \mathbf{m}_j), \ i = 1, \dots, n. \end{aligned} \tag{6.10}$$

Here ρ_i denote the densities, $\mathbf{m}_i$ the momenta, p_i the partial pressures, and M_i, λ_{ij} are mobility constants and Maxwell–Stefan coefficients.
We investigate global existence of smooth solutions to the system (6.10). In certain flow regimes, e.g. late time and large mobilities, the Maxwell–Stefan system converges to a parabolic limit system. For weakly coupled systems we prove this fact in a relative entropy framework for diffusive relaxation in one space dimension. As a tool for efficient 1D simulations in such regimes, we present an asymptotic preserving scheme.

AMS Subject Classification: 35L65, 35A01.

On Potential Methods for Porous Media Flows

W. Wendland (Universität Stuttgart) 15:40

This lecture presents some joint work with Mirela Kohr (Babe s Bolyai Univ., Cluj–Napoca), Massimo Lanza de Cristoforis (Univ. Padua) and Sergey E. Mikhailov (Brunel University, Uxbridge) We obtain existence and uniqueness results in Sobolev spaces for transmis- sion problems for the nonlinear Darcy–Forchheimer–Brinkman system in a Lipschitz domain and the linear Stokes system in the exterior in R 3 and also on compact Riemannian manifolds. We apply a layer potential method for the Stokes and Brinkman systems combined with a fixed point argument to obtain existence. Uniqueness is also obtained for sufficiently small given data.

S 14 : Applied analysis

Tuesday 16:30 - 18:30 Weimar hall, Large hall

Corrector estimates for a class of imperfect transmission problems

S. Reichelt (Weierstrass Institute for Applied Analysis and Stochastics) 16:30

Based on previous homogenization results for imperfect transmission problems in two-component domains with periodic microstructure, we derive quantitative estimates for

the difference between the microscopic and macroscopic solution. This difference is of order ε^ρ, where $\varepsilon > 0$ describes the periodicity of the microstructure and $\rho \in (0, \frac{1}{2}]$ depends on the transmission condition at the interface between the two components. The corrector estimates are proved without assuming additional regularity for the local correctors using the periodic unfolding method.

Effective models for two bulk-regions separated by a thin layer including nonlinear transmission conditions

M. Gahn (Friedrich-Alexander-Universität Erlangen-Nürnberg), M. Neuss-Radu (Friedrich-Alexander-Universität Erlangen-Nürnberg), P. Knabner (Friedrich-Alexander-Universität Erlangen-Nürnberg) 16:50

We consider a system of nonlinear reaction–diffusion equations in a domain consisting of two bulk regions separated by a thin layer Ω_ϵ^M with a periodic heterogeneous structure. The thickness of the layer Ω_ϵ^M is of order ϵ, and the equations inside the layer depend on the parameter ϵ. The diffusion in the thin layer is of order ϵ^γ with an additional parameter $\gamma \in [-1, 1]$, which describes the size of the diffusion. On the interface between the bulk regions and the layer a nonlinear Neumann-boundary condition is assumed, i. e. the normal flux depends on the solutions on both sides of the interface. For $\epsilon \to 0$, i. e. the thin layer reduces to an interface Σ between two bulk regions, macroscopic problems with effective transmission and boundary conditions are derived, the solution of which approximates the thin layer model. The critical part is the derivation of limit equations for the thin layer. For this purpose, the method of two-scale convergence and the unfolding operator in thin domains is used. The macroscopic model depends on the choice of γ. For $\gamma = 1$ the effective transmission conditions are described by local reaction–diffusion problems on the interface Σ, where for $\gamma \in (-1, 1)$ we obtain an ordinary differential equation on Σ and for $\gamma = -1$ a reaction–diffusion equation on Σ with homogenized diffusion coefficients.

A two-scale Stefan problem arising in a model for tree-sap exudation

I. Konrad (Simon Fraser University), M. Peter (Universität Augsburg), J. Stockie (Simon Fraser University) 17:10

The study of tree-sap exudation, in which a (leafless) tree generates elevated stem pressure in response to repeated daily freeze–thaw cycles, gives rise to a multiscale problem involving heat and multiphase liquid/gas transport. By assuming a periodic cellular structure based on an appropriate reference cell, we derive a homogenized heat equation governing the global temperature on the scale of the tree stem, with all the remaining physics relegated to equations defined on the reference cell. The particular form of our homogenized temperature equation is obtained using periodic-homogenization techniques with two-scale convergence, which we apply rigorously in the context of a simpler two-phase Stefan-type problem corresponding to a periodic array of melting cylindrical ice bars with a constant thermal diffusion coefficient. Numerical simulations are performed to validate the results and draw conclusions regarding the phenomenon of sap exudation.

Analysis of chemotactical biofilm growth in evolving microstructures

R. Schulz (Friedrich-Alexander-Universität Erlangen-Nürnberg) 17:30

The talk is concerned with the growth of biofilms made by chemotactical bacteria within a saturated porous media. The increase of a biomass on the surface of the solid matrix changes the porosity and impede the flow through the pores. By formal periodic homogenization we derive an averaged model describing the process via Darcy's law and upscaled transport equations with effective coefficients given by the evolving microstructure at the pore-scale. Based on the assumption of uniform evolve of the underlying pore geometry and slight self-diffusivity of the bacteria, solvability in a weak sense global in time or at least up to a possible clogging phenomenon is shown. Furthermore, by assuming sufficient regularity on the data we prove boundedness of the solution.

Weak-mild solution to microscopic simplified Multiple Myeloma model

F. Klawe (Institute of Applied Mathematics, Heidelberg University) 17:50

Our research is directed to describe evolution of cancer cells concetration in moving domain $\Omega(t)$. The motivation for the following work is multiple myeloma, which is a cancer of plasma cells. We study model, which describe evolutions of cancer cell's concentration (inside the domain), concentration of osteoblast (surface component, which is responsible for changing the bone structure) and changes of bone's structure (shape of domain).

We consider a case of circular geometry, i.e. let $\Omega(0)$ be a circle and changes of its geometry are uniform in all directions. $\Gamma(t)$ is a boundary of $\Omega(t)$ and its evolution is defined by ODE on radius of $\Omega(t)$. Then we consider the following system of equations

$$\begin{cases} \dfrac{\partial u}{\partial t} - \Delta u = F_u(u) & x \in \Omega(t),\ t \in [0,T], \\ \dfrac{\partial u}{\partial \vec{n}} + Vu = F_\gamma(u,B) & x \in \Gamma(t),\ t \in [0,T], \\ \dfrac{\partial B}{\partial t} + BVH - \Delta_\Gamma B = F_B(u,B) & x \in \Gamma(t),\ t \in [0,T], \\ \dfrac{dR(t)}{dt} = V(t) = g(\overline{B})(R_{\max} - R(t))(R(t) - R_{\min}), \end{cases} \tag{6.11}$$

where V is normal velocity of the boundary and H stays for mean curvature of $\Gamma(t)$, that is $H(t) = \frac{1}{R(t)}$. Additionally, we assume that the velocity of boundary depends on radius $R(t)$ and mean value of surface's concentration, i.e. $\overline{B} = \frac{1}{|\Gamma(t)|}\int_{\Gamma(t)} B \,\mathrm{d}S$, see [3]. Similar problem was considered e.g. in [2], where authors study the flow of an incompressible fluid through a porous medium with hydrophile granules. However, there was no surface component and surface moves only in one direction. General information about equations defined on moving surfaces may be found in [1].

We present proofs of existence, regularity and uniqueness to (6.11). This is joint work with A. Marciniak-Czochra and A. Mikelić.

[1] G. Dziuk and C.M. Elliott. Finite element methods for surface PDEs. Acta Numer. 22:289–396, 2013.

[2] A. Fasano and A. Mikelić. The 3D flow of a liquid through a porous medium with absorbing and swelling granules. Interfaces and Free Boundaries, 4:329 – 261, 2002.

[3] B.P. Ayati and C.M. Edwards and G.F. Webb and J.P. Wikswo A mathematical model of bone remodeling dynamics for normal bone cell populations and myeloma bone disease. Biol Direct., 2010, 5–28

S 14 : Applied analysis

Wednesday 14:00 - 16:00 Coudraystr. 13B, Ground floor, Lecture hall 3

Structured deformations and applications

M. Morandotti (Technische Universität München) 14:00

In this talk, I shall introduce the theory of first- and second-order structured deformation and present some results concerning the relaxation of energy functionals in the context of structured deformations. Applications to some specific problems will also be discussed.

A Non rank One convexity result involving logarithmic strain measures

I. Ghiba (Alexandru Ioan Cuza University of Iași), P. Neff (University of Duisburg-Essen), R. Martin (University of Duisburg-Essen) 14:20

It is known that the $F \mapsto \|\log U\|^2$ and $F \mapsto \|\mathrm{dev}_n \log U\|^2$ are not rank-one convex at arbitrary $F \in \mathrm{GL}^+(2)$. Here, $\log U$ is the principle matrix logarithm and $U = \sqrt{F^T F}$ is the stretch tensor, while $\mathrm{dev}_n \log U = \log U - \frac{1}{n} \log U$. The term $\|\log U\|^2$ arises naturally as the geodesic distance of F to the group of rotations $\mathrm{SO}(2)$. Therefore, it is tempting to formulate elastic strain energies $W = W(F)$ in terms of the "geodesic" strain measure $\|\log U\|^2$ or $\|\mathrm{dev}_n \log U\|^2$ by setting $W(F) = \Psi(\|\log U\|^2)$ or $W(F) = \widetilde{\Psi}(\|\mathrm{dev}_n \log U\|^2)$, respectively. We investigate the existence of such type of energies which are rank-one convex.

Rank-one convexity implies polyconvexity in isotropic planar incompressible elasticity

I. Ghiba (Alexandru Ioan Cuza University of Iași), R. Martin (University of Duisburg-Essen), P. Neff (University of Duisburg-Essen) 14:40

We study convexity properties of energy functions in plane nonlinear elasticity of incompressible materials and show that rank-one convexity of an objective and isotropic elastic energy W on the special linear group $\mathrm{SL}(2)$ implies the polyconvexity of W.

On approximation of finite-energy sequences of Muller's functional with non-standard 2-well potential

A. Raguz (Zagreb School of Economics and Management) 15:00

We present the basic results and conjectures regarding possibility of approximation of finite-energy sequences of Müller's functional (which was for the first time, and in its simplest form, studied in paper S. Müller: Singular perturbations as a selection criterion for periodic minimizing sequences, Calc. Var. Partial Differential Equations 1(2) 169–204 (1993)) by 1-Lipschitz and 1-periodic finite-energy sequences. Our results extend known results in the case of simplest pinning term concerning the actual minimizers as small parameter epsilon tends to zero, whereby standard assumption on growth of 2-well potential at infinity (which immediately yields equi-coercivity) is replaced by non-standard one.

A vanishing viscosity analysis for a two dimensional ferroelectricity model

Y. Luo (Universität Kassel) 15:20

A ferroelectric model is considered. Ferroelectric models include the behavior of the polarization in ferroelectric materials. A material is called ferroelectric if it has a spontaneous polarization which can be reversed by the application of an electric field. In this case, a hysteresis curve is present. We use a convex dissipation functional, which is positively homogeneous of degree one, to model such hysteresis effects. This leads to a model that belongs to the class of rate-independent systems. An existence result of energetic solutions is already given in a paper by Mielke/Timofte. Since jumps occur as early as possible in the context of energetic solutions, we use as an alternative vanishing viscosity approach to obtain a viscosity solution, where the jumps occur as late as possible. Some sufficient conditions on the domain and the coefficients are given and the existence of viscous solutions is shown by means of a time discretization approach. At the end of the talk, we will give a preview of the solution concepts by pushing the viscosity term to zero.

Tikhonov Funtionals Incorporating Tolerances

P. Gralla (University of Bremen), I. Piotrowska-Kurczewski (University of Bremen), P. Maaß (University of Bremen) 15:40

Tikhonov functionals are a well known method for solving inverse problems. They consist of a discrepancy and a penalty term. The first term evaluates the deviation of simulated data from measured data. We alternate this term by incorporating tolerances, which neglects small deviations from the data within a prescribed tolerance. This approach adapts ideas from support vector regression, which utilizes such a tolerance for identity operators and semi discrete problems. Furthermore, the application for inverse problems is motivated by applications where such tolerances naturally occur, e.g. application with multiple measurements. In this case instead of one measurement a confidence interval for the measurement can be used. In this work we provide an overview on the necessary analysis and alternation of Tikhonov functionals incorporating tolerances. In addition,

example of applications are shown and discussed.

S 14 : Applied analysis

Wednesday 16:30 - 18:30 Coudraystr. 13B, Ground floor, Lecture hall 3

Quantitative homogenization in non-linear elasticity

M. Schäffner (TU-Dresden), S. Neukamm (TU Dresden) 16:30

We consider a nonlinear elastic composite with a periodic micro-structure described by the non-convex integral functional

$$I_\varepsilon(u) = \int_\Omega W\left(\frac{x}{\varepsilon}, \nabla u(x)\right) - f(x)\cdot u(x)\,dx,$$

where $u : \Omega \to \mathbb{R}^d$ is the deformation, $f : \Omega \to \mathbb{R}^d$ is an external force, $\varepsilon > 0$ denotes the size of the micro-structure, and $W(y, F)$ is a stored energy function which is periodic in y. As it is well-known, under suitable growth conditions, I_ε Γ-converges to a functional with a homogenized energy density $W_{\text{hom}}(F)$, which is given by an *infinite-cell formula*. Under appropriate assumptions on W and on the microstructure, we show that in a neighbourhood of $SO(d)$, the set of rotations, the homogenized stored energy function W_{hom} is of class C^2 and characterized by a *single-cell homogenization formula*. Moreover, for small data, we establish an estimate on the homogenization error, which measures the distance between (almost) minimizers u_ε of I_ε and the minimizer of the homogenized problem. More precisely, we prove that the L^2-error as well as the H^1-error of the associated two-scale expansion decays with the rate $\sqrt{\varepsilon}$.

A quantitative two-scale expansion in stochastic homogenization

S. Neukamm (TU Dresden) 16:50

We study linear elliptic systems with rapidly oscillating, random (stationary and ergodic) coefficients. We consider the classical two-scale expansion for such systems and establish an H^1-error estimate in the case of coefficients with arbitrarily slow-decaying correlations. The talk is based on a joint work with Antoine Gloria and Felix Otto.

Stochastic Unfolding

M. Heida (WIAS Berlin), S. Neukamm (TU Dresden), M. Varga (TU Dresden) 17:10

The aim of our work is to provide a simple homogenization procedure for energy driven problems involving stochastic rapidly-oscillating coefficients. Our intention is to extend the approach used in the periodic unfolding method to the stochastic setting. Specifically, we recast the notion of stochastic two-scale convergence in the mean by introducing a convenient stochastic unfolding operator. This operator admits similar properties as the

periodic unfolding operator, leading to an uncomplicated homogenization method.

Asymptotic modelling of the wave-propagation over acoustic liners

A. Semin (Technische Universität Berlin), K. Schmidt (BTU Cottbus-Senftenberg & Technische Universität Berlin) 17:30

We will consider the acoustic wave propagation in a channel separated from a chamber by a thin periodic layer. This model stand for microperforated absorbers which are used to supress reflections from walls. Due to the smallness of the periodicity a direct numerical simulation, e.g. with the finite element method (FEM), is only possible for very large costs. Based on homogenization techniques we find impedance transmission conditions, which integrated into numerical methods like the FEM or the boundary element method leads to much lower computational costs. For liners of finite length their endings have a significant impact to the macroscopic absorption and this effect is a-priori not considered with the transmission conditions. We aim to describe the interaction of the thin periodic layer with the singularities from its endings asymptotically when the periodicity and layer thickness δ tend to zero. For this, the Kondratiev theory for corner singularities (which is based on the Mellin transform) has to be extended to infinite cones with periodic layers in the spirit of Nazarov.

Perturbation analysis of hyperbolic PDAEs describing gas networks

C. Huck (Humboldt-Universität zu Berlin) 17:50

Hyperbolic partial differential algebraic equations play an important role in the modelling of gas networks. We rely on an isothermal simplification of the Euler equations to model the behaviour of pressure and mass flow in pipes that are coupled by a set of perturbed balance equations

$$\begin{aligned} \mathfrak{u}' + \mathcal{B}\mathfrak{u} + \mathcal{R}(\mathfrak{u}, t) &= \delta_\Omega \\ C_r \mathfrak{u}_r + C_\ell \mathfrak{u}_\ell &= \mathfrak{u}_\Gamma + \delta_\Gamma. \end{aligned}$$

Here, $\mathfrak{u}_r$ and $\mathfrak{u}_\ell$ denote the pressures and flows at the left and right ends of the pipes, $\mathfrak{u}_\Gamma$ denotes the boundary and coupling data of the network. δ_Ω are perturbations along the pipes and δ_Γ are perturbation at the nodes.
By considering function spaces on graphs and the application of a suitable homogenization technique, we can reduce the above system and focus the perturbation analysis on a system of PDEs of the form

$$\begin{aligned} \mathfrak{u}' + \mathcal{B}\mathfrak{u} + \mathcal{R}(\mathfrak{u}, t) &= \mathcal{F}(0, \mathfrak{u}_\Gamma, \mathfrak{u}'_\Gamma) \\ \mathfrak{u}^{\delta'} + \mathcal{B}\mathfrak{u}^\delta + \mathcal{R}(\mathfrak{u}^\delta, t) &= \mathcal{F}(\delta_\Omega, \mathfrak{u}_\Gamma + \delta_\Gamma, \mathfrak{u}'_\Gamma + \delta'_\Gamma) \end{aligned}$$

We present perturbation estimates that are strongly linked to the perturbation index for partial differential algebraic equations.

S 14 : Applied analysis

Thursday 14:00 - 16:00 Coudraystr. 13B, Ground floor, Lecture hall 3

Electrothermal description of organic semiconductor devices by p(x)-Laplace thermistor models

A. Glitzky (Weierstrass Institute for Applied Analysis and Stochastics) 14:00

Large-area organic LEDs for lighting applications show a spatially inhomogeneous luminance at high power caused by inhomogeneous current flow and electrothermal feedback. In this talk we study a stationary $p(x)$-Laplace thermistor model describing the electrothermal behavior of organic semiconductors taking into account non-Ohmic current-voltage laws and self-heating effects. The coupled system consists of a current-flow equation for the electrostatic potential and a heat equation with a source term resulting from Joule heating and having a priori only L^1-integrability. The self-heating in the device is modeled by an Arrhenius-like temperature dependency of the electrical conductivity. The non-Ohmic electrical behavior is described by a power law such that the electrical conductivity depends nonlinearly on the electric field. The consideration of spatial substructures with different power laws gives rise to a $p(x)$-Laplace-type problem with discontinuous exponent.
In this talk we present joint work with M. Bulíček (Prague), J. Fuhrmann and M. Liero (both WIAS Berlin). We report on the solvability of the $p(x)$-Laplace thermistor model, regularity and boundedness properties of its solutions and discuss some numerical aspects.

The entropy method for a reaction-diffusion system modelling band-trapped states

M. Kniely (Karl-Franzens-Universität Graz), K. Fellner (Karl-Franzens-Universität Graz) 14:20

A semiconductor is basically characterised by two energy levels. The lower one is referred to as the valence band, and the upper one as the conduction band. By a sufficient amount of energy, electrons can be transferred from the lower to the upper energy level. Band-trapped states correspond to intermediate energy levels between the valence band and the conduction band. In this talk, we first discuss the reason for considering trapped levels and introduce an appropriate reaction-diffusion system. Next, we will review the so-called entropy approach used to obtain an entropy entropy-dissipation inequality. A major part of the talk shall also focus on the derivation of this EED-inequality itself. At the end, exponential convergence to the equilibrium will be proven.

An entropic gradient structure Lindblad equations

M. Mittnenzweig (WIAS Berlin), A. Mielke (WIAS Berlin) 14:40

We show that all Lindblad equations (i.e. quantum Markov semigroups) on a finite-

dimensional Hilbert space satisfying a detailed balance condition possess a gradient flow structure with respect to the relative von Neumann entropy. The corresponding Riemannian metric for the density matrices can be viewed as a non-commutative analog of the 2-Wasserstein metric for probability distributions. This is joint work with Alexander Mielke.

Gradient flow formulation and longtime behaviour of a constrained Fokker-Planck equation

S. Eberle (Universität Duisburg-Essen), B. Niethammer (Universität Bonn), A. Schlichting (Universität Bonn) 15:00

We consider a Fokker-Planck equation which is coupled to an externally given time-dependent constraint on its first moment. This constraint introduces a Lagrange-multiplier which renders the equation nonlocal and nonlinear. The model arises in the thermodynamic modeling of many-particle storage systems, such as for example Lithium-ion batteries.
First, we exploit an interpretation of this equation as a Wasserstein gradient flow of a free energy $\mathcal{F}$ on a time-constrained manifold. From this interpretation, we sketch how to prove existence of solutions by passing to the limit in an explicit Euler scheme obtained by minimizing $h\mathcal{F}(\varrho)+W_2^2(\varrho^0,\varrho)$ among all ϱ satisfying the constraint for some ϱ^0 and time-step $h>0$.
Second, we provide quantitative estimates for the rate of convergence to equilibrium when the constraint converges to a constant. The proof is based on the investigation of a suitable relative entropy with respect to minimizers of the free energy chosen according to the constraint. The rate of convergence can be explicitly expressed in terms of constants in suitable logarithmic Sobolev inequalities. (arXiv: 1612.01427)

Gamma-convergence and relaxations for gradient flows in metric spaces: a minimizing movement approach

F. Fleißner (Technische Universität München) 15:20

In [1], we present new abstract results on the interrelation between the minimizing movement scheme for gradient flows along a sequence of Γ-converging functionals and the gradient flow motion for the corresponding limit functional, in a general metric space. We are able to allow a relaxed form of minimization in each step of the scheme, and so we present new relaxation results too.

[1] Florentine Fleißner, Gamma-convergence and relaxations for gradient flows in metric spaces: a minimizing movement approach, Submitted. *arXiv preprint:1603.02822* (2016)

Overdamped limit of the Vlasov-Fokker-Planck equation: A variational approach

A. Lamacz (TU Dortmund) 15:40

Coarse-graining is the procedure of approximating a complex system by a simpler or lower-dimensional one, often in some limiting regime. Coarse-graining limits are by nature singular limits. Therefore rigorous proofs of such limits typically hinge on exploiting certain structural features of the equations such as variational-evolution structures, which, for instance, are present in gradient flows.
In this talk we introduce and discuss such a variational structure arising from the theory of large deviations for stochastic processes. We show how in systems, which are characterized by a large deviation rate functional, passing to a limit is facilitated by the dual formulation of the rate functional, in a way that interacts particularly well with coarse-graining. Being closely related to classical variational methods for gradient flows, our approach is also applicable to systems with non-dissipative effects. As an example we use the technique to derive the large friction (overdamped) limit of the Vlasov-Fokker-Planck equation.
The talk is based on a joint work with M. Hong Duong, Mark A. Peletier and Upanshu Sharma.

S 14 : Applied analysis

Thursday 16:30 - 18:30 Coudraystr. 13B, Ground floor, Lecture hall 3

Unfolding in fractional order Sobolev and Bessel spaces, application to the homogenization of Coulomb-contact on periodic cracks

J. Orlik (Fraunhofer ITWM) 16:30

We consider the elasticity problem in a heterogeneous domain with a periodic microstructure with contact on multiple open cracks in a simply connected domain. The contact is described by the Signorini and Coulomb-friction conditions. Problem is nonlinear, the dissipative functional depends on the unknown solution and the existence of the solution is usually proven by the fix-point argument in the Sobolev spaces with a little higher regularity, $H^{1+\alpha}$ (see [2]). We want to homogenize the contact problem: rescale all the estimates, who are necessary for the compactness proof and pass to the limit. We estimate the co-normal derivatives from above by definition and from below using the equations. The entering constants are from the trace, inverse trace and Korn's inequalities, which should be rescaled. For the rescaling of all these inequalities we use the unfolding technique, introduced in [1] and extend it to the fractional order Sobolev (like in [3]) and Bessel-potential spaces here.

[1] D. Cioranescu, A. Damlamian and G. Griso, Periodic unfolding and homogenization, C. R. Acad. Sci. Paris, Sér. I, 335, 2002, 99–104.

[2] C. Eck, J. Jarusek, Krbec, Unilateral Contact Problems: Variational Methods and Existence Theorems, Springer, 2005.

[3] M. Gahn, P. Knabner & M. Neuss-Radu, Homogenization of reaction-diffusion processes in a two-component porous medium with a nonlinear flux condition at the interface, and application to metabolic processes in cells, Preprint Angew. Math., Uni Erlangen, No. 384, 2014

Homogenization and dimension reduction for a textile shell. A priori estimates

S. Wackerle (Fraunhofer ITWM), G. Griso, J. Orlik (Fraunhofer ITWM) 16:50

A model of a woven textile as a three dimensional elasticity problem with contact between yarns is considered. After starting with the microscopic representation of the reference textile we use the decomposition of displacements for beams [1, 2] to account for the beam-like structure [4] of a single fiber. Two approaches for the decomposition of displacements of beams, leading to the linear or the non-linear shell-models in the limit, are presented and justified. Additionally, we show the idea of how to extract the plate-behavior with the help of the extra information hidden in te contacts and verify them by the resemblance to the decomposition of a plate [1, 3]. Especially, the von-Karman plate model as transition between the linear and nonlinear case is discussed.

[1] G. Griso. Decomposition of displacements of thin structures. J. Math. Pures Appl. 89 (2008), 199-233.

[2] Blanchard, Dominique and Griso, Georges. Decomposition of deformations of thin rods: Application to nonlinear elasticity. Analysis and Applications 07 (2009), 21-71.

[3] Blanchard, Dominique and Griso, George. Decomposition of the Deformations of a Thin Shell. Asymptotic Behavior of the Green-St Venant's Strain Tensor. Journal of Elasticity 101 (2010), 179-205.

[4] G. Griso. Asymptotic behavior of structures made of curved rods. Analysis and Applications. 6, 01 (2008), 11-22.

Homogenization and Design optimization for a periodic heterogeneous plate under a given constraint

M. Hauck (Fraunhofer ITWM), J. Orlik (Fraunhofer ITWM) 17:10

The design optimization problems for heterogeneous elastic plates arise in many different applications, for instance in filters under local bending. We consider a plate with an in-plane periodic structure under a local point-bending moment or force. We employ basic homogenization techniques for linear periodic heterogeneous plates and pass to the anisotropic Kirchhoff-Love plate in the limit, where the effective bending coefficients were obtained from the auxilliary bending unit experiments on the periodicity cell by averaging of the local moments of outer-plane stresses. Since the plate structure is made

of beam, we use the beam-FE method for solving the cell-problems. We homogenize the plate and then find an analytic solution under the local bending perturbation. Our further aim is to minimize the deflection caused by a localized load in the effective anisotropic plate. For that case we need to define a design space, which takes into account the constraint of anisotropy. We provide a particular example, where we can show how the design parameters influence the maximal plate deflection.

Some Basic Boundary Value Problems for Plane Theory of Elasticity of Porous Cosserat Media with Triple-Porosity

B. Gulua (Iv. Javakhishvili Tbilisi State University, Department of Mathematics), R. Janjgava (I. Vekua Institute of Applied Mathematics of Iv. Javakhishvili Tbilisi State University) 17:30

The static equilibrium of porous elastic materials with Triple-Porosity is considered in the case of an elastic Cosserat medium. The corresponding three-dimensional system of differential equations is derived. Detailed consideration is given to the case of plane deformation. A two-dimensional system of equations of plane deformation is written in the complex form and its general solution is represented by means of two analytic functions of a complex variable and four solutions of Helmholtz equations. The constructed general solution enables one to solve analytically a sufficiently wide class of plane boundary value problems of the elastic equilibrium of porous Cosserat media with Triple-Porosity. The concrete boundary value problems for a concentric ring is solved.

Acknowledgements:
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Averaging of time-periodic dissipation potentials in rate-independent processes

M. Heida (WIAS Berlin), A. Mielke (WIAS Berlin) 17:50

We study the existence and well-posedness of rate-independent systems (or hysteresis operators) with a dissipation potential that oscillates in time with period ε. In particular, for the case of quadratic energies in a Hilbert space, we study the averaging limit $\varepsilon \to 0$ and show that the effective dissipation potential is given by the minimum of all friction thresholds in one period, more precisely as the intersection of all the characteristic domains. We show that the rates of the process do not converge weakly, hence our analysis uses the notion of energetic solutions and relies on a detailed estimates to obtain a suitable equi-continuity of the solutions in the limit $\varepsilon \to 0$.

Self-similar solutions for Smoluchowski's coagulation equation with time-dependent tails

M. Bonacini (Universität Bonn), B. Niethammer (Universität Bonn), J. Velázquez 18:10

Smoluchowsi's coagulation equation is a nonlocal integral equation used to describe

irreversible mass aggregation phenomena. A key question in the analysis of this model is whether the long-time behaviour of solutions is universal and described by special self-similar solutions. In this talk I present some recent progress on this topic: in particular, I discuss an existence result of a new one-parameter family of self-similar solutions with time-dependent tails, for a class of rate kernels homogeneous of degree one. Such solutions are characterised in terms of their precise asymptotic behaviour at infinity.

S 14 : Applied analysis

Friday 09:00 - 11:00 Coudraystr. 13B, Ground floor, Lecture hall 3

Global existence results for viscoplasticity

A. Mielke (WIAS Berlin) 09:00

We study a model for rate-dependent gradient plasticity at finite strain based on the multiplicative decomposition of the strain tensor, and investigate the existence of global-in-time solutions to the related PDE system. We reveal its underlying structure as a \emph{generalized gradient system}, where the driving energy functional is highly nonconvex and features the geometric nonlinearities related to finite-strain elasticity as well as the multiplicative decomposition of finite-strain plasticity. Moreover, the dissipation potential depends on the left-invariant plastic rate and thus, depends on the plastic state variable.
We introduce the notion EDI solutions that fulfill the energy-dissipation inequality on suitable time intervals. The construction of solutions follows De Giorgi's minimizing movement scheme and is based on variational interpolants. The crucial point is to establish the closedness of the marginal Fr\'{e}chet subdifferential that contains the plastic backstresses, which is highly nonlinear and non-monotone set-valued mapping.
This is joint work with Riccarda Rossi (Brescia) and Giuseppe Savar\'e (Pavia).

The effect of forest dislocations on the evolution of a phase-field model for plastic slip

S. Wojtowytsch (Durham University), P. Dondl (Albert-Ludwigs-Universität Freiburg), M. Kurzke (The University of Nottingham) 09:20

We consider a phase field model for dislocations introduced by Koslowski, Cuitino, and Ortiz in 2002. The model describes a single slip plane and consists of a Peierls potential penalizing non-integer slip and a long range interaction modeling elasticity. Forest dislocations are introduced as a restriction to the allowable phase field functions: they have to vanish at the union of a number of small disks in the plane. Garroni and Müller proved large scale limits of these models in terms of Gamma-convergence, obtaining a line-tension energy for the dislocations and a bulk term penalizing slip. This bulk term is a capacity stemming from the forest dislocations.

In the present work, we show that the contribution of the forest dislocations to the the viscous gradient flow evolution is small. In particular it is much slower than the timescale for other effects like elastic attraction/repulsion of dislocations, which, by recent results due to del Mar Gonzales and Monneau/Patrizi and Valdinoci is already slower than the time scale from line tension energy. Overall, this leads to an effective behavior like a gradient flow in a wiggly potential. On the other hand, of course, when adding a driving force in the direction of increasing slip, one needs to spend the energy to overcome the obstacles. The forest dislocations thus act like a dissipation for increasing slip, but their effect on the propagation is absent for decreasing slip.

On the existence of minimisers for strain-gradient single-crystal plasticity

K. Anguige (Albert Ludwigs Uni Freiburg) 09:40

We discuss the existence of minimisers for a family of energy-minimisation problems related to the single-slip-to-single-plane relaxation of single-crystal, strain-gradient elastoplasticity with L^p-hardening penalty in 3 dimensions. In these relaxed models, where only one slip-plane normal can be activated at each material point, the main challenge is to show that the energy of geometrically necessary dislocations is lower-semicontinuous along bounded-energy sequences which satisfy the single-plane condition, meaning precisely that this side condition should be preserved in the weak-L^p limit. This is done with the aid of an 'exclusion' lemma of Conti & Ortiz, which allows one to put a lower bound on the dislocation energy at interfaces of (single-plane) slip patches, thus precluding fine phase-mixing in the limit. The key ideas of the proof will be illustrated by considering a simplified 2-dimensional model of elastoplasticity.

On local minimizers of prestrained thin elastic rods

M. Cicalese (Technische Universität München), M. Ruf (Technische Universität München), F. Solombrino (Technische Universität München) 10:00

We study the stable configurations of a thin three-dimensional weakly prestrained rod subject to a terminal load as the thickness of the section vanishes. We derive a one-dimensional limit theory and show that isolated local minimizers of the limit model can be approached by local minimizers of the three-dimensional model. We focus on isotropic materials and a two-layer prestrained three-dimensional model for which the limit energy further simplifies to that of a Kirchhoff rod-model of an intrinsically curved beam. In this case we study the stability of the straight configuration. Our analysis shows that at a critical load the intrinsic curvature makes the straight configuration unstable. If time permits we show the emergence of helical/hemihelical local minimizers at the critical load both in the 1d and 3d model.

Asymptotic rigidity and homogenization of layered materials with stiff components

C. Kreisbeck (Universiteit Utrecht), F. Christowiak (Universität Regensburg) 10:20

In the context of finite-strain elastoplasticity, we investigate the effective behavior of variational models for bilayered composite materials featuring large elastic constants in one component. Our particular interest lies in understanding whether the presence of the stiff layers forces a rigid macroscopic material response. The answer to this question is expected to depend on the scaling relation between stiffness and layer thickness.
In this talk, we characterize the limit deformations of sequences of uniformly bounded energy as the thickness of the layers tends to zero, and identify two different scaling regimes. If the elastic constants diverge sufficiently fast, the observed macroscopic deformations coincide with those in the special case of completely rigid layers. As it is shown in a previous preprint, the latter correspond exactly to global rotations of shear deformations in layer direction, provided they are locally volume preserving. One major step in the proof is to quantify the layer stiffness with the help of the geometric rigidity estimate established by Friesecke, James, and Müller in 2002. To show optimality of this regime, an explicit construction of a family of deformations based on bending of the individual stiffer layers is given, which yields macroscopically softer material behavior. These findings serve as a basis for proving a rigorous homogenization result via Γ-convergence.

S 15: Uncertainty Quantification

Organizers: Martin Eigel (WIAS Berlin)
Elisabeth Ullmann (TU München)

S 15 : Uncertainty Quantification

Tuesday 14:00 - 16:00 Weimar hall, Seminar room 5
Chair: Elisabeth Ullmann (TU München)

PDE-constrained optimization under uncertainty using low-rank methods

P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems), S. Dolgov, A. Onwunta, M. Stoll (MPI Magdeburg) 14:00

We discuss optimization and control of unsteady partial differential equations (PDEs), where coefficients in the PDE as well as the control may be uncertain. This may be due to the lack of knowledge about the exact physical parameters like material properties describing a real-world problem (epistemic uncertainty) or the inability to apply a computed optimal control exactly in practice. Using a stochastic Galerkin space-time discretization of the optimality system resulting from such PDE-constrained optimization problems under uncertainty leads to a large-scale linear or nonlinear system of equations in saddle point form. Nonlinearity is treated with a Picard-type iteration in which linear saddle point systems have to be solved in each iteration step. Using data compression based on separation of variables and tensor train (TT) format, we show

how these large-scale indefinite and (non)symmetric systems that typically have 10^8 to 10^{11} unknowns can be solved without the use of HPC technology. The key observation is that the unknown and the data can be well approximated in a new block TT format that reduces complexity by several orders of magnitude. As examples, we consider control and optimization problems for the linear heat equation, the unsteady Stokes and Stokes-Brinkman equations, as well as the incompressible unsteady Navier-Stokes equations. The talk reviews the results published in [1, 2] and provides new results for the Navier-Stokes case.

[1] P. Benner, A. Onwunta, M. Stoll, Block-diagonal preconditioning for optimal control problems constrained by PDEs with uncertain inputs, *SIAM Journal on Matrix Analysis and Applications*, 37(2):491–518, 2016.

[2] P. Benner, S. Dolgov, A. Onwunta, M. Stoll, Low-rank solvers for unsteady Stokes-Brinkman optimal control problem with random data, *Computer Methods in Applied Mechanics and Engineering*, 304:26–54, 2016.

Structured polynomial chaos for uncertain optimal control problems with fast sensitivity generation and sparsity exploitation

L. Bergner (Universität Heidelberg), C. Kirches (Technische Universität Braunschweig) 14:40

We present advances in structure-exploiting non-intrusive polynomial chaos (PC) methods for the numerical solution of nonlinear optimal control problems with parametric uncertainties. In particular, we make use of the special structure induced by the spectral projection to reuse model derivatives and exploit sparsity information leading to a fast automatic sensitivity generation. This greatly reduces the computational load of Newtontype methods for the solution of the resulting high-dimensional PC-surrogate problem. The results are complemented by a complexity comparison and a numerical case study.

Topology Optimization under Uncertainties

J. Neumann (Weierstrass Institute for Applied Analysis and Stochastics) 15:00

A novel approach for risk-averse structural topology optimization under uncertainties is presented which takes into account random material properties and random forces. For the distribution of material, a phase field approach is employed which allows for arbitrary topological changes during optimization. The state equation is assumed to be a high-dimensional PDE parametrized in a (finite) set of random variables.
For the examined case, linearized elasticity with a parametric elasticity tensor is used. Instead of an optimization with respect to the expectation of the involved random fields, for practical purposes it is important to design structures which are also robust in case of events that are not the most frequent. As a common risk-aware measure, the Conditional Value at Risk (CVaR) is used in the cost functional during the minimization procedure. The arrising stochastic equations are solved with the robust Monte Carlo method.

Sparse Collocation for Functions of Countably Many Gaussian Random Variables

O. Ernst (TU Chemnitz), B. Sprungk (TU Chemnitz), L. Tamellini (CNR-IMATI Pavia) 15:20

We present and analyze sparse grid collocation approximations of Hilbert space-valued functions depending on countably many Gaussian random variables. Such functions appear as weak solutions or quantities of interest associated with elliptic PDEs with lognormal diffusion coefficients. We outline a general L^2-convergence theory based on previous work by Bachmayr et al. [1] and Chen [2] and establish an algebraic convergence rate for sufficiently smooth functions of countably many variables. We verify specifically convergence for sparse grid collocation employing Gauss-Hermite nodes and also show an algebraic convergence w.r.t. the resulting number of sparse grid points for this case. Numerical experiments illustrate our theoretical results.

[1] M. Bachmayr, A. Cohen, R. DeVore, and G. Migliorati, *Sparse polynomial approximation of parametric elliptic PDEs. part II: lognormal coefficients*, ESAIM Math. Model. Numer. Anal., (2016).

[2] P. Chen, *Convergence analysis of an adaptive sparse quadrature for high-dimensional integration with Gaussian random variables.* arXiv:1604.08466, 2016.

[3] O. G. Ernst, B. Sprungk and L. Tamellini, *Convergence of sparse collocation for functions of countably many Gaussian random variables - with application to lognormal elliptic diffusion problems.* arXiv:1611.07239, 2016.

Investigation of a Global Adaptive Sampling Method Based on Least-Square Support Vector Regression

M. Steiner (Bauhaus-Universität Weimar), T. Lahmer (Bauhaus-Universität Weimar), J. Bourinet (SIGMA Clermont) 15:40

In many engineering fields, a global sensitivity analysis of the model seems to be advantageous since it provides a basis to judge on the parameters' importance; nevertheless, it needs numerous data points and correspondingly, considerable amount of computational costs. A common technique to overcome this problem is to use the so-called metamodels with which the necessary data can be extremely reduced by the use of a smaller support sample set and the approximation of the remaining points. There are many papers about different model choices and optimal sampling strategies (e.g. [1], [2]). However, often more sample points have to be added if the required quality of the approximation is not reached. In the fields of reliability analysis and optimization, there are numerous adaptive sampling methods to add new points to an existing approximation. Nevertheless, those are local methods because just some areas are interesting regarding this research fields. In contrast, related to the global sensitivity analysis, we are interested in the global behaviour of the originally engineering problems and accordingly in global adaptive sampling methods. In this contribution one new global adaptive sampling

method based on a special metamodel – the least-squares support vector regression – is presented.

[1] A. Forrester, A. Sobester, A. Keane. Engineering design via surrogate modelling: A practical guide. Progress in Aerospace Sciences, Wiley (2008)
[2] T. Most, J. Will. Metamodel of Optimal Prognosis - an Automatic Approach for Variable Reduction and Optimal Metamodel Selection. Tagesband der Weimarer Optimierungs- und Stochastiktage 5.0 (2008)

S 15 : Uncertainty Quantification

Tuesday 16:30 - 18:30 Weimar hall, Seminar room 5
Chair: Martin Eigel (WIAS Berlin)

Multilevel Subset Simulation for Rare Events

R. Scheichl (University of Bath) 16:30

In this talk I will present a multilevel conditional estimator for rare event probabilities. The underlying approach has been proposed in several communities under various names. We will base our work on the methodology proposed by [Au & Beck, 2001] in the engineering community under the name of *subset simulation*. In statistics, it is sometimes referred to as *importance splitting*. It has also strong links to sequential Monte Carlo methods and so-called *shaking transformations* [Gobet & Liu, 2015].
Our proposed estimator uses different model resolutions and varying numbers of samples on the hierarchy of failure sets. We construct the failure sets such that a high number of samples are used when the model evaluations are cheap, while only using a small number of expensive samples, in order to reduce the computational cost. A key idea in our new estimator is the use of a posteriori error estimation to guarantee the critical subset property that may be violated when changing model resolution from one failure set to the next. The error estimators also allow to avoid expensive calculations for samples that are far away from the boundary of our failure sets. The computational gains are demonstrated on a model elliptic PDE with random coefficients. Some possible extensions to other applications will also be given.
This is joint work with Daniel Elfverson (UmeåUniversity).

A comparison of Markov Chain Methods for Reliability Estimation

C. Proppe (Karlsruher Institut für Technologie (KIT)) 17:10

Subset simulation is a successful method for reliability estimation, especially if small failure probabilities or problems involving a high-dimensional vector of random variables are involved. In subset simulation, intermediate threshold levels for the response quantity are introduced that define a nested subset of less rare events. The failure probability

is then computed as the product of larger probabilities that require sampling from conditional distributions. These samples are generated from ergodic Markov chains (MC). While subset simulation requires a low number of nested subsets only, a generalization in the sense of particle methods has been proposed recently, where a threshold is associated to each sample, samples are moved to new positions in the design space and the number of moves for the initial samples to reach the failure region are counted and yield an estimator for the failure probability. The algorithm allows for an easy parallel implementation. Just as for subset simulation, sampling from conditional distributions is required when moving a particle. The MC algorithm for moving a particle requires a burn-in period which increases the number of response evaluations drastically in order to maintain independence of the particles. In contrast, for subset simulation, it is argued that a burn-in period is not necessary. However, the reasoning is based solely on stationarity of the MC and problems with as well as remedies against low acceptance rates of the MC algorithm are discussed in the literature on subset simulation. In this presentation, the influence of a burn-in period and possible remedies against low acceptance rates is investigated for both subset simulation and particle methods. Moreover, application of surrogate models based on Kriging and low-rank approximations, resp., is investigated to further reduce the number of response evaluations.

Metropolis-Hastings Importance Sampling estimator

D. Rudolf (Georg-August-Universität Göttingen), B. Sprungk (TU Chemnitz) 17:30

We propose a Metropolis-Hastings Importance Sampling estimator for the approximation of expected values w.r.t. partially known probability measures, such as posterior distributions. The method is asymptotically correct and numerical experiments indicate that it outperforms classical Markov chain Monte Carlo based on the Metropolis-Hastings algorithm.

Multilevel Monte Carlo approximation of functions

S. Krumscheid (EPFL), F. Nobile (EPFL) 17:50

Many applications across sciences and technologies require a careful quantification of non-deterministic effects to a system output, for example aiming to evaluate the system's reliability or to gear it towards more robust operation conditions. At the heart of these considerations lies an accurate yet efficient characterisation of uncertain system outputs. For the approximation of moments of said outputs, the multilevel Monte Carlo method has been established as a computationally efficient sampling method that is applicable to a wide range of applications. While a characterisation of the uncertain output in terms of a few moments may be sufficient in some applications, many applications would, however, require many (possibly infinitely many) moments for an accurate approximation of an output's distribution. That is, a moment-based characterisation of an uncertain output (e.g. via a truncated Edgeworth series expansion) is often unfeasible. As a matter of fact, in some practically relevant cases, for example when the system output follows a

Lévy distribution (also known as a van der Waals profile), moments do not even exist, so that a moment-based characterisation is even impossible here.
In this talk we will introduce novel multilevel Monte Carlo techniques for an efficient characterisation of an uncertain system output's distribution. These techniques rely on accurately approximating general parametric expectations, i.e. expectations that depend on a parameter, uniformly on some interval. The resulting multilevel Monte Carlo estimators of such functions enable to derive efficient approximations of various means to characterise a system output's distribution, for example an approximation to the characteristic function or to the cumulative distribution function. A further important consequence of these results is that they enable the construction of multilevel Monte Carlo estimators for various robustness indicators, such as for quantiles (also known as value-at-risk) or for the conditional value-at-risk. It is noteworthy that these robustness indicators cannot be expressed as moments. Consequently, they had been out of reach for an efficient treatment via standard multilevel Monte Carlo methods thus far. Here, we will present the construction and the analysis of these multilevel Monte Carlo methods for functions and discuss their applications to the estimation of robustness indicators. Moreover, we will illustrate the performance of the developed multilevel methodologies using different benchmark examples, before, if time permits, addressing problems arising in the context of robust design in aeronautics.

Inverse uncertainty quantification based on a test bench hardware

*P. Glaser (*Robert Bosch GmbH), M. Schick* (*Robert Bosch GmbH), K. Petridis* (*Robert Bosch GmbH), V. Heuveline** (**University Heidelberg)* 18:10

Many industrial applications involve model parameters for which correct values are rarely available in a precise way. To get a better characterization of those parameters, they are expressed by stochastic variables instead of deterministic values. Those stochastic variables can be considered as parameter uncertainties and hence, they have a significant impact on simulation results. The quantification of such uncertainties plays a crucial role, for example, in face of unknown component tolerances or measurement errors. Among many others, one challenging task is to infer knowledge on parameter distributions in light of experimental data.
In this context, Bayesian inference offers a framework to combine numerical simulations with observed experimental data to infer better knowledge on model parameter uncertainties. A standard method is the so-called Markov Chain Monte Carlo (MCMC) approach in which the posterior of the model parameters is updated using correlated Monte Carlo samples. However, MCMC often converges very slow, such that usually many samples are required to achieve a high numeric accuracy. This is a large drawback, especially if the numerical cost of a single simulation becomes prohibitive. Surrogate models, like, for example, Polynomial Chaos (PC) expansions, can significantly reduce the number of required samples. They are a meta description of model output variations with respect to the random input which enables a quick and numerical cheap exploration of the posterior distribution.

Furthermore, we built a test bench hardware, which is used to measure a motor characteristic of an electric drive with uncertain physical parameters. In our test bench it is possible to define physical reference parameter distributions a priori and store an according set of measurements. This can be viewed as an equivalent representation of series production fluctuation of electric drives. We use this reference data to compute the posterior distribution obtained from the MCMC approach using a PC surrogate model. Starting from a prior distributions, which are different to the distributions taken to generate our reference data. Our focus is on the validation of the method based on real measurements from an industrial application. The numerical results shows that the PC approach with MCMC can reduce significantly the required computation time compared to MCMC on the original simulation model by consistent results.

S 15 : Uncertainty Quantification

Wednesday 14:00 - 16:00 Coudraystr. 13B, 2nd floor, Room 208
Chair: Martin Eigel (WIAS Berlin)

Solving high-dimensional problems in uncertainty quantification by hierarchical tensor representations

R. Schneider (TU Berlin) 14:00

Hierarchical Tucker tensors or tree tensor networks offer stable and robust approximations of high order tensors and multi-variate functions by a low order cost. For many high dimensional problems, including uncertainty quantification via parametric PDE's etc., this approach has the potential to circumvent from the curse of dimensionality. For numerical computations, the high-dimensional parametric PDEs is cast into an optimization problem constraint by restricting to set of tensors of bounded multilinear ranks $\mathbf{r}$. For an approximation by elements from this highly nonlinear subset, we focus on a Galerkin framework. The underlying admissible set is no longer convex, but it is an algebraic variety. We consider various optimization methods, e.g. Riemannian optimization and corresponding gradient schemes, and projection methods by hard and soft thresholding based on the Hierarchical SVD (HSVD). Numerical examples include the solution of the forward problem in uncertainty quantification, inverse Bayesian computation (see the talk by Marschall et al.) and Langevin dynamics in molecular dynamical systems. We may discuss further randomized algorithms for low rank tensor regression, sampling techniques and tensor completion.

Bayesian Inversion using Hierarchical Tensors

M. Marschall (WIAS Berlin), R. Schneider (TU Berlin), M. Eigel (WIAS Berlin) 14:40

Bayesian inverse problems have been tackled with a variety of sampling methods for a long time. Despite steady progress, also modern variants of classical MCMC still

converge rather slowly by nature and critically depend on an appropriate choice of algorithm parameters. Well-known surrogate models from UQ (e.g. polynomial chaos) can be employed to at least speed up the sampling process. However, also a complete functional treatment of the involved probability densities is feasible, entirely avoiding any MC sampling and explicitly representing the posterior measure in terms of some functional basis. The proposed sampling-free approach will be discussed in the context of hierarchical tensor representations which are employed for the adaptive evaluation of a random PDE (the forward problem) and the subsequent high-dimensional quadrature of the log-likelihood.

Hierarchical Matrix Techniques for Uncertainty Quantification of PDE on Random Domains

J. Dölz (Universität Basel), H. Harbrecht (Universität Basel) 15:00

We are interested in the first and second moment of the solution of PDE with random input data. Previous works have shown that these moments can be computed by the hierarchical matrix arithmetic in almost linear time if the solution depends linearly on the data. However, in the case of random domains the dependence of the solution of the data is nonlinear. Extending previous perturbation approaches we can linearize the problem and can compute the first moment up to third order accuracy and the second moment up to second order accuracy in almost linear time.

Comparison of parametric and non-parametric methods for bladed disks with random geometric mistuning

M. Koebele (Karlsruher Institut für Technologie (KIT)), C. Proppe (Karlsruher Institut für Technologie (KIT)) 15:20

Bladed disks give an example of systems where structural geometric uncertainties drastically influence the dynamical behavior. Indeed, small random deviations in the geometry of blades arising during the manufacturing process inevitably break the cyclic periodicity of the disk, since the blades are no longer identical. This is referred to as geometric mistuning and can lead to a spatial confinement of vibration energy in certain blades, in which a significant increase in forced-response vibration amplitudes will occur compared to the tuned system.

In order to quantify this phenomenon for industrial bladed disks, geometric random uncertainties are firstly implemented in a finite element model via random modifications of the nodal coordinates of the reference mesh. Parametric method consists then in building a reduced-order model, in which reduced structural matrices directly depend on all parameters related to the random geometry of the blades. Non-parametric method builts also a reduced-order model, but structural reduced matrices are randomly generated using the maximum entropy principle regardless of the blade geometry. The dispersion parameters controlling the random generation of the structural matrices are however estimated as a function of the geometric tolerances.

In this work, we compare the results of both approaches. The advantages and the

disadvantages of each method will be discussed.

Fuzinsumo - Fuzzy investigation with surrogate models

T. Oberleiter (Friedrich-Alexander-Universität Erlangen-Nürnberg), K. Willner (FAU Erlangen-Nürnberg) 15:40

In our contribution, we investigate the accuracy of surrogate models of fuzzy systems. Within a virtual tolerance analysis, unknown uncertainties are considered by fuzzy numbers. These fuzzy numbers consist of higher-dimensional intervals, where each interval assigned a membership value. To reproduce fuzzy numbers correctly, a large number of system evaluations is needed. Instead of performing numerically expensive full systems, we employ surrogate models with radial basis functions. In order to find sufficiently accurate surrogate models with as few as possible sampling points, we investigate the influence of the sampling points on the respective intervals of fuzzy numbers. As an example, we investigate the tilting of an x-ray aperture, which shows different accuracy for different sampling strategies. The reference results for the nonlinear multi-body system are calculated by a Matlab optimizer and are compared with the results of the surrogate models.

S 15 : Uncertainty Quantification

Wednesday 16:30 - 18:30 Coudraystr. 13B, 2nd floor, Room 208
Chair: Elisabeth Ullmann (TU München)

Deterministic Continuation and CERES for Stochastically Forced PDEs

C. Kühn (TU München) 16:30

In this talk I shall illustrate an approach to study the dynamics of stochastic PDEs (or more generally stochastic dynamical systems) with respect to parameters using deterministic continuation methods. In particular, I shall focus on the case of local fluctuations for the stochastic Allen-Cahn equation and explain the practical implementation as well as a novel framework for Combined ERror EStimates (CERES). This is joint work with Patrick Kürschner (MPI Magdeburg).

Quadrature and sampling methods for linear dynamical systems with uncertain parameters

R. Pulch (Ernst-Moritz-Arndt-Universität Greifswald) 16:50

We consider linear dynamical systems consisting of ordinary differential equations or differential algebraic equations. An output of the system is defined as a quantity of interest. The systems include physical parameters, which are often affected by uncertainties due to modelling errors or measurement errors, for example. We substitute the parameters by random variables to obtain an uncertainty quantification. The quantity of

interest becomes a random process, which can be expanded into a series with orthogonal basis functions depending on the parameters and time-dependent coefficient functions. For example, polynomial chaos expansions apply orthogonal polynomials determined by the probability distribution. Either intrusive methods, like the stochastic Galerkin scheme, or non-intrusive methods, like quadrature rules and sampling techniques, yield approximations of the unknown coefficient functions.
In this talk, we investigate the non-intrusive approach. Both quadrature rules and sampling methods are defined by a set of nodes in the parameter domain and an associated set of real-valued weights. Now the linear dynamical systems have to be solved for each node. We analyse a quadrature technique using an auxiliary linear system, where all those linear dynamical systems are collected into a large system. The auxiliary system is only weakly coupled by the application of a single input to all subsystems and merging the outputs of the subsystems. The large system features own properties like the Hankel norm and the Hardy norms of its transfer function with respect to the input-output-behaviour. This information allows for conclusions on the accuracy and characteristics of the underlying quadrature rule or sampling method. Furthermore, model order reduction is applicable to the auxiliary system, although the original linear dynamical system may be relatively small.
We demonstrate results of numerical computations for a test example. For instance, linear dynamical systems are obtained by the mathematical modelling of electric circuits or mechanical mass-spring-damper configurations.

Map-based stochastic turbulence modeling

H. Schmidt (BTU Cottbus - Senftenberg) 17:10

Direct numerical simulation (DNS) can investigate fundamental problems in fluid mechanics since it solves the governing equations without further assumptions. Novel alternatives are stochastic approaches like the one-dimensional-turbulence model (ODT) [1] and multi-dimensional Eulerian (e.g. ODTLES) and Lagrangian extensions that incorporate ODT-type models [2, 3, 4]. The ability to resolve molecular processes (as DNS) distinguishes ODT and ODTLES from techniques such as large eddy simulation (LES). The ODTLES model turns into a DNS or into a stand-alone ODT in the respective distinguished limit. In the talk we illustrate the potential of these stochastic approaches by comparing various results against DNS and experiments, see e.g. [4, 5, 6, 7, 8, 9].

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[2] Schmidt, H. and Klein, R. (2003). A generalized level-set/in-cell-reconstruction approach for accelerating turbulent premixed flames, *Combustion Theory and Modelling*, **7**, 243-267

[3] Gonzalez-Juez, E. D., Schmidt, R. C., Kerstein, A. R., ODTLES simulation of wall-bounded turbulent flows, *Physics of Fluids*, **23**, 125102, 2011

[4] Glawe, C., Gonzalez-Juez, E. D., Schmidt, H., Kerstein, A.R., ODTLES simulations of turbulent flows through heated channels and ducts, 8th International Symposium on Turbulence and Shear Flow Phenomena, Poitiers, France, 2013

[5] F. Schulz, C. Glawe, H. Schmidt, A. R. Kerstein, Toward modeling of CO_2 multiphase flow patterns using a stochastic multi-scale approach, *Environmental Earth Sciences*, **70**, 3739–3748, 2013

[6] Schmidt, H., Kerstein, A.R., Nédélec, R., Wunsch, S., Sayler, B. J. (2013). Numerical simulation of a laboratory analog of radiatively induced cloud-top entrainment, *Theoretical and Computational Fluid Dynamics*, **27**, 377-395

[7] Z. Jozefik, A. R. Kerstein, H. Schmidt, S. Lyra, H. Kolla, J. H. Chen (2015). One-dimensional turbulence modeling of a turbulent counterflow flame with comparison to DNS, *Combustion and Flame*, **162**, 2999-3015

[8] Z. Jozefik, A. R. Kerstein, H. Schmidt, (2015). Simulation of shock-turbulence interaction in non-reactive flow and in turbulent deflagration and detonation regimes using one-dimensional turbulence, *Combustion and Flame*, **164**, 53-67

[9] A. Movaghar, M. Linne, M. Oevermann, F. Meiselbach, H. Schmidt, Alan R. Kerstein (2016). Numerical investigation of turbulent-jet primary breakup using One-Dimensional Turbulence, *International Journal of Multiphase Flow*, **89**, 241-254

Macroscopic models for investigation of the dynamics of foam structures

E. Kancheva (TU Bergakademie Freiberg), A. Ams (TU Bergakademie Freiberg) 17:30

In the presentation the dynamics of open-cell foam structures will be discussed. Measurements of real foam structures were carried out by computer tomography (CT) and afterwards they were analyzed statistically. By correlation and spectral analysis the investigated samples have been modeled with stochastic processes. Based on the dynamical model the eigenfrequencies have been calculated. Various types of load has been applied to the generated foam structures – for example – harmonical excitation and white noise. The frequency response functions and the time solutions have been calculated.

S 15 : Uncertainty Quantification

Friday 09:00 - 11:00 Coudraystr. 11C, Lecture hall 1

Ensemble Kalman Filter for Inverse Problems

C. Schillings 09:00

Many problems in the physical sciences require the identification of unknown parameters from indirect observations. We will discuss a Bayesian approach to the inverse problem, which allows quantifying the uncertainty in the unknown parameters.
To solve the inverse problem, we will focus on ad hoc methods, in particular the Ensemble Kalman Filter (EnKF). These methods are widely and successfully used by practitioners in cases where the model evaluations are prohibitively expensive. The low computational costs, the straightforward implementation and their non-intrusive nature make them appealing in various areas of application, but, on the downside, they are underpinned by very limited theoretical understanding. We will present an analysis of the EnKF based on the continuous time scaling limits, which allows studying the properties of the EnKF for a fixed ensemble size.The theoretical considerations give useful insights into properties of the methods and provide tools for a systematic development and improvement.
This is joint work with Andrew M. Stuart (Caltech) and part of the EPSRC-funded project EQUIP.

Quantifying stochastic influences in biomedical imaging

P. Zaspel (Universität Basel) 09:40

Medical imaging is one of the important tools for diagnostics in a clinical environment. In the specific field of cancer diagnosis, radiological imaging is one of the only non-invasive ways to decide whether tissue is stemming back from cancer or not. However, images taken by Magnetic Resonance Tomography (MRT) or Computed Tomography (CT) devices are subject to high variabilities due to imaging errors, patient movement, etc. In the recent years, the extraction of features or meta-data from radiological images is a growing research topic. Ultimately, this data shall be assembled to imaging biomarkers, i.e. numbers, which shall be reliable diagnosis indicators for (non-)existence of tissue with cancer. However, these biomarkers are assumed to be subject to a high variability based on the underlying image variability. The purpose of our ongoing research endeavour is to find ways to quantify the reliability of imaging biomarkers.
In the recent years, we have introduced the meshless kernel-based stochastic collocation using radial basis functions. This non-intrusive UQ method is designed to solve large-scale problems in a high-order convergent and scaling fashion. It combines high-order algebraic or even exponential convergence rates of spectral (sparse) tensor-product methods with optimal pre-asymptotic convergence of kriging and the profound stochastic framework of Gaussian process regression.
We are about to integrate our stochastic collocation approach into the appropriate imaging tool pipeline of radiologists. In our presentation, we will give the latest results on the described developments.

Optimal Sensor Placement for Data Assimilation Problems

I. Riedel (TU Chemnitz), R. Herzog (TU Chemnitz) 10:00

We consider state and parameter estimation in thermo-elastic models. The goal is to estimate the displacement in a certain point from temperature measurements, which is

motivated from an engineering application. To make this estimation more robust, we simultaneous estimate uncertain parameters to keep the model up-to-date. Therefore we use self-calibrating data assimilation techniques. The quality of the estimation depends strongly on the position of the measurement devices. We present optimal experimental design techniques for such data assimilation problems to get the optimal sensor positions.

Identification of a Visco-plastic Model with Uncertain Parameters using Bayesian Methods

E. Adeli (Institute of Scientific Computing), E. Adeli (Institute of Scientific Computing) 10:20

The evaluation of the performance of engineering structures includes models of behavior of materials, structural elements, loadings, external excitations etc. In assessment studies, there are several classes of uncertainty related to the lack of information on loading conditions/excitations, behavior of material properties over time, geometry and boundary conditions which may be identified and reduced by the means of quality control or system monitoring and identification.

In this work the focus is on the propagation of the uncertainty into a visco-plastic model and quantification of the uncertainty in the response of the model described by model parameter uncertainty. To do so, Stochastic Finite Element Method (SFEM) is applied for different tests e.g. relaxation test and creep test. Once the forward model, which is a much more realistic model than the discrete model, is provided, in order to identify the model parameters, solving the inverse problem is studied. Employing some Bayesian approaches like Polynomial Chaos Expansion based update, leads us to update and identify the model parameters which are set as uncertain values in the first step. The results confirm the efficiency of the used methods.

S 16: Optimization

Organizers: Michael Stingl (Friedrich-Alexander-Universität Erlangen-Nürnberg)
Gerd Wachsmuth (TU Chemnitz)

S 16 : Optimization

Tuesday 14:00 - 16:00 Weimar hall, Seminar room 4
Chair: Michael Stingl (Friedrich-Alexander-Universität Erlangen-Nürnberg)

Topology and material orientation optimization of anisotropic material based on evolution equations

D. Jantos (Institute of Mechanics of Materials, Ruhr-Universität Bochum), P. Junker (Institute of Continuum Mechanics, Ruhr-Universität Bochum), K. Hackl (Institute of Mechanics of Materials, Ruhr-Universität Bochum) 14:00

The general objective of topology optimization is to find a mechanical structure with maximized stiffness by minimizing the work of external forces for given boundary conditions [1]. For an anisotropic material, the distribution of mass density within a given model space and the local orientation of the material can be considered as design variables. We solve this problem by introducing a variational problem for the field of the mass density to describe the topology of the mechanical structure and Euler angles to describe the local material orientation in the three-dimensional space [2]. The mass density and the Euler angles are both defined by internal variables and by minimizing the Gibbs free energy according to Hamilton's principle in dynamics for dissipative processes [3], we are able to find evolution equations for all internal variables. The evolution equations describe the change of the internal variables within time (i.e. steps of an iterative process) towards the optimal solution. We introduce a Lagrange multiplier to control the total mass within the model space and apply a natural-like growth for the structure mass [4] while the local material orientation will be optimized simultaneously. The numerical solution can be obtained within a solitary finite element environment, where the the internal variables are defined at the Gaußpoints. A regularization with a discontinuous Galerkin approach for the internal variable enables us to suppress the well-known checkerboarding phenomena without any further filtering while evaluating the evolution equations within each finite element separately [5]. Therefore, the density field and the Euler angles describing the material orientation are no additional field unknowns and can be calculated locally which strongly reduces the calculation effort. Finally, we present solutions of optimized structures for different boundary problems to show the potential of our model.

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[2] Junker, Philipp. A novel approach to representative orientation distribution functions for modeling and simulation of polycrystalline shape memory alloys. International Journal for Numerical Methods in Engineering (2014)

[3] Junker, Philipp and Hackl, Klaus. A variational growth approach to topology optimization. Structural and Multidisciplinary Optimization (2015)

[4] Jantos, Dustin R. and Junker, Philipp and Hackl, Klaus. An evolutionary topology optimization approach with variationally controlled growth. Computer Methods in Applied Mechanics and Engineering (2016)

[5] Junker, Philipp and Hackl, Klaus. A discontinuous phase field approach to variational topology optimization. Structural and Multidisciplinary Optimization (2016)

Optimization of topology and shape combining phase-field modelling and discrete stochastic algorithms

A. Keller (Karlsruher Institut für Technologie (KIT) - Institut für Baustatik), I. Münch (KIT), W. Wagner (Karlsruher Institut für Technologie) 14:20

For the design of structures in civil engineering we are interested in an approach to combine topology and shape optimization. Therefore, we use a phase-field model to generate topology first. Second, shape optimization with stochastic methods is performed. Shape optimization typically works in a subset of allowable shapes having fixed topological properties, e.g. the number of holes within a structure. Thus, topology optimization generates the design concept and shape optimization fine-tunes a chosen design. Both methods have strengths and weaknesses such that we work out a concept to circumvent latter.

Our topology optimization is not limited by an initial structure, as often found in literature. We start with a homogeneously filled region of material without holes and reduce the filling degree of material. Depending on the desired filling degree, internal length scale, and nucleation parameter, the final topology differs. For low filling degree of material, the topology typically results in framework structures with more or less trusses.

Note, that it is not possible to estimate the overall fitness of obtained topologies concerning more complex criteria required in civil engineering. Hence, we use metaheuristic shape optimization as the second step, in particular genetic optimization and ant algorithm, respectively. These methods can easily consider constraints from stress and displacement conditions. Additionally, in the phase-field model we cannot simulate hinges, which can be implemented in shape optimization. In other words, the shape optimization is the bridge to practical tasks in civil engineering.

Objective Functions for the Shape Optimization of Temperature Control Channels in High-Pressure Die Casting

M. Frings (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), M. Behr (RWTH Aachen University, Chair for Computational Analysis of Technical Systems), S. Elgeti (RWTH Aachen University, Chair for Computational Analysis of Technical Systems) 14:40

High-pressure die casting is a well known process in the field of aluminum processing. The quality of the produced cast parts highly depends on the die quality. An important ingredient for high-quality casting dies is the design of the temperature control channels. The state-of-the art approach is as follows: Several boreholes are drilled from the sides through the die. They are afterwards plugged to form closed flow channels. This classic approach has a few disadvantages: (1) The flow behavior inside the flow channels is not optimal due to sharp edges, and (2) it is hard to bring the channels close to the cavity and fit them to the shape of the cast part. One possible remedy to these drawbacks is offered by additive manufacturing methods, such as selective laser melting. Becoming increasingly affordable, they allow for free-form flow channels that result in much better flow properties of the temperature control liquid. In addition, one can use numerical optimization to find an optimal channel design. The latter is the purpose of the underlying work.

A requirement for numerical optimization is an appropriate objective function. This contribution presents several objective functions that are promising candidates for a numerical shape optimization. In plastics injection moulding, numerical optimization is already used in the industry (c.f., [1]). Due to the very different material behavior of plastic and aluminum, objective functions cannot be copied from the plastics manufacturing process. Therefore, in this contribution, new objective functions for the high-pressure die casting are developed. They are evaluated w.r.t. their sensitivity and their relation to the desired goals of the process. This includes not only average temperatures and temperature deviation, but also more economically driven objectives, like cycle time.

An exemplary die proposed in [2] serves as reference for the evaluation. Partners from the RWTH Aachen foundry institute are using this die for experiments. Thus, it is possible to verify optimization results experimentally.

[1] D. E. Dimla, M. Camilotto and F. Miani. Design and optimisation of conformal cooling channels in injection moulding tools. Journal of Materials Processing Technology, 164–165:1294–1300, 2005.

[2] R. Siegbert, et al. Individualized production in die-based manufacturing processes using numerical optimization. The International Journal of Advanced Manufacturing Technology, 80:851-859, 2015

Exploration of Internal Response Sensitivities of Materially Nonlinear Structures

J. Liedmann (TU Dortmund University), F. Barthold (TU Dortmund University) 15:00

In the context of structural design optimisation, the structural response and the structural design sensitivities have to be determined in order to use gradient based mathematical optimisation. Barthold [1] proposed an approach to compute response sensitivities analytically by means of variational principles. The approach is based on an enhanced concept of kinematics, that offers rigorous separation of geometry and physics. Thus, implicit dependencies arise not until global equilibrium is defined. The approach allows simultaneous determination of structural response and response sensitivities within a finite element framework. Sensitivities and subsequent discretisations can be derived easily, see [2]. Central part of this approach is the computation of pseudo load and sensitivity matrices.
The advantages of the aforementioned approach has been shown for material nonlinearities, like elastoplasticity in [5]. In this case, it is necessary to store and analyse the deformation history, due to the path-dependent material behaviour. The approach of internal variables has proven successful in this context. Additional to the computation of pseudo load and sensitivity matrices, the sensitivities of these internal variables have to be determined as well. This yields a history sensitivity matrix, see [4].
The term *internal structure of sensitivities* is introduced in [3] and is an abbreviation of eigen- and singluar values and vectors, as well as corresponding spectra of pseudo load and sensitivity matrices. This information is provided by means of singular value decomposition (SVD). The examination of sensitivity matrices utilising SVD is called *design exploration* and provides deep insight into sensitivity information. It also hints on major and minor influence of design variables on structural response.
The idea of design exploration in the context of structural design sensitivity analysis considering elastoplastic material behaviour is outlined. Numerical and algorithmic implementation is presented and demonstrated in selected numerical examples in the context of structural shape optimisation.

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[2] Barthold, F.-J. et al.: Mathematical Modelling and Optimization of Complex Structures. Springer International Publishing. Chap. Efficient Variational Design Sensitivity Analysis, pp. 229-257. (2016)

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[4] Liedmann, J. and Barthold, F.-J.: Optimisation of structures with inelastic deformations, PAMM 16(1):703-704. (2016)

[5] Wiechmann, K.: Theorie und Numerik zur Berechnung und Optimierung von Strukturen mit elastoplastischen Deformationen, Dissertation. LU Hannover (2001)

optimization of arch dam with robust analysis

T. Fengjie (ISM / BUW) 15:20

Considering the previous design experience of the arch dams, the use of shape-optimization of this type of dams can effectively reduce the cost of construction and utilize the properties of construction materials to the best way. To apply the shape-optimization, suitable variables were chosen to formulate the objective function, i.e. to minimize the volume of the arch dam. Additionally, a series of constraints are derived together with a reasonable and convenient penalty function has been formed. This function can easily enforce the characteristics of constraints and optimal design. For the optimization method, a Genetic Algorithm is adopted to perform a global searching. One of the used constraints in the current study is employed to fulfill requirements of the structural safety. Therefore, a reliability analysis was applied to attain both the safety and service life of arch dam. By means of this, the key factors, that influence the stability an safety of arch dam, significantly can be acquired, and supply a good way to take preventive measures to prolong ate the service life of the arch dams and enhances the safety of the structure.

S 16 : Optimization

Tuesday 16:30 - 18:30 Weimar hall, Seminar room 4
Chair: Gerd Wachsmuth (TU Chemnitz)

Solving Lipschitz continuous, piecewise smooth problems by LiPsMin: Results and extensions

S. Fiege (Paderborn University), A. Walther (Paderborn University), A. Griewank (Yachaytech) 16:30

LiPsMin is a minimization algorithm for Lipschitzian, piecewise smooth problems. All nondifferentiablilities of the considered objective functions are caused by abs(), min() and max(). This is a reasonable assumption, since objective functions of this form are typical for many applications from both academia and the real world, i.e., minimax problems from robust optimization.
The idea of the method is to locate optima by successively generating piecewise linearizations and minimizing them by exploiting the polyhedral decomposition of the domain caused by the nondifferentiable points. The piecewise linearization can be computed in its abs-normal-form by minor extension of standard algorithmic differentiation tools. Further information about the PL and the abs-normal form can be found in *Griewank, On stable piecewise linearization and generalized algorithmic differentiation, Optimization Methods and Software, 2013.*
One key ingredient of LiPsMin is the efficient exploitation of structure while solving the local subproblems. In *Griewank, Walther, Fiege, Bosse. On Lipschitzian optimization based on gray-box piecewise linearization. Mathematical Programming, 2015* a bundle type method was introduced for this purpose. But other approaches are possible as indicated in *Griewank, Walther. First- and second-order optimality conditions for piecewise smooth functions, Optimization Methods and Software, 2016* and are discussed

in this talk. Furthermore, numerical results are analyzed and a comparison is made between LiPsMin and other state-of-the-art nonsmooth software tools.

Gradient sampling methods on Riemannian manifolds and algebraic varieties

S. Hosseini, A. Uschmajew (University of Bonn) 16:50

Gradient sampling (GS) is a conceptually simple method for optimization of locally Lipschitz functions. The idea is to approximate the subdifferential at a given point by a convex hull of randomly sampled nearby gradients. We consider generalizations of this approach to optimization problems posed on complete Riemannian manifolds or closed algebraic varieties admitting an a-regular stratification. The latter scenario is motivated by optimization problems on low-rank matrices or tensors. The main task is to prove that the minimum norm element in a convex hull of vectors, which are obtained by transporting Riemannian gradients from nearby points to the current tangent space, is a descent direction with respect to a retraction, provided that the number of sampled gradients equals at least the dimension of the manifold/variety plus one. For varieties it is further necessary to discuss what should happen in the singular points, where one may be faced with a tangent cone that is not convex. Under reasonable assumptions, we are able to prove that with probability one the limit points of our proposed GS algorithms are Clarke stationary points relative to their strata. Numerical experiments illustrate that the approach can be useful, e.g., for finding sparse vectors in a subspace or for low-rank matrix denoising.

Open-source tool-chain for optimal input design for dynamical systems

S. Mayr, G. Grabmair 17:10

Protoframe GUI is a Scilab extension developed at the University of Applied Sciences Upper Austria. It was developed to create a free framework and front-end for semi-automated matching of real and virtual prototypes. The ideal model-based development process is characterized among other things by a permanent comparison between virtual and real prototypes. The industrial practice shows, however, that due to variations in parameters, simulation and test results often differ significantly from each other. Due to high costs, repeated comparisons between model and reality are often neglected. The objective was the development of professional expertise, infrastructure and resources for largely automated comparison of mechatronic systems as a precondition for model-based control design methods and any kind of realistic simulation of complex structures (e.g., lifetime optimization, lightweight). To carry out the semi-automated matching of parameters based on real prototypes two groups of methods were developed and implemented in our modular software platform. On the one hand the automatic parameter identification based on test responses and on the other hand the generation of optimal excitation signals. In order to cover a wide range of industrial relevant mechatronic applications, the domains of solid mechanics (multi-body systems), thermo-mechanics and power electronics are also taken into account. To support the design process and to visualize the results, a graphical front-end was implemented. In this paper, we focus on the generation

of optimal excitation signals for dynamical systems using Protoframe GUI. The goal is to generate input signals with high information content to ensure e.g. accurate parameter estimation and additionally consider (mechanical) boundary conditions. Therefore, standard optimal control, a common practice to generate trajectories for mechanical systems, is extended by an input design approach.
After this introduction Section **??** discusses briefly the basic principles of input design and trajectory generation implemented in our tool. In Section **??** the optimal input design part of the developed tool-chain is presented to the reader, followed by a simulation experiment in Section **??**. Conclusions are drawn in Section **??**.

Optimal Expansion Planning for an Electric Distribution Network with the NLP Solver WORHP

A. Berger (Universität Bremen), F. Jung (Universität Bremen), M. Echim (Universität Bremen), C. Büskens (Universität Bremen), M. Schollmeyer (IAV GmbH) 17:30

Electrical distribution networks of today form very complex systems. Simul- taneously, the integration of renewable energies makes it essential to continu- ously expand the existing networks. This leads to the necessity of an automated optimal expansion planning. In this contribution, we show our method to find the optimal expansions for an existing network. This is done by calculating the power flow equations as con- straints of a nonlinear optimisation problem (NLP). To find an optimal solution with respect to several objective functions, we use the diameters of the exist- ing lines as degrees of freedom. The problems are solved with the NLP solver WORHP which is designed to exploit sparse structures resulting from the power flow equations for instance. We show the functionality of the presented method by applying it to a real distribution network.

SmartFarm - Data based optimization for optimal energy management

F. Jung (University of Bremen), C. Büskens (Universtität Bremen) 17:50

In Germany the renewable energy law determine the boundary conditions, when renewable energy production is profitable. Every company in Germany is affected by this law. We focus on the agriculture sector, particularly on small and medium size farms. They are special in a way that they have an enormous consumption of electricity and they are not that highly invested like the huge farms.
In the project SmartFarm we develop a method that automatically decides which renewable energies are profitable to use at the farm for the next hours. To this means optimisation methods are used on various levels.
Initially, all necessary data is measured on a demonstration object. This data forms the basis for data based learning methods for the modelling of the consumers (e.g. milk cooling), the producers (e.g. solar plant) and the energy storage systems (e.g. battery storage device). In this talk we will focus on the data based models of the producers and energy storage systems. Optimisation methods are used to identify optimal parameters for a general ansatz function, which is derived from a Taylor approximation.

Building on highly accurate models an optimization regarding the own consumption of the produced electricity is realised. That means the farm should use as much as possible of the self-generated energy instead of buying electricity from the public grid. Taking all details into account this results in a highly complex stochastic, mixed-integer nonlinear optimisation problem. A transformed but still non-linear problem can be solved by the NLP-solver WORHP.
We develop all models with real data of the demonstration object and can verify them with this data as well. First results and the further course of action will be discussed in the talk.

S 17: Applied and numerical linear algebra

Organizers: Sara Grundel
Karsten Kahl (Bergische Universität Wuppertal)

S 17 : Applied and numerical linear algebra

Tuesday 14:00 - 16:00 Coudraystr. 11C, Room 202

Analysis of linear data fitting approaches for multiple observations

I. Hnetynkova (Charles University, Prague) 14:00

In many areas, there is a need to solve linear approximation problems of the form

$$AX \approx B,\ A \in \mathcal{R}^{n\times m},\ B \in \mathcal{R}^{n\times d},$$

where A is a linear model and the columns of the right-hand side B represent multiple observations (measurements) being available on this model. Classical linear data fitting approaches such as various variants of the least squares method (called also regression or errors-in-variables modeling) can be generalized to this setting. For example, when the errors are present both in the model matrix A and the observation matrix B, the total least squares (TLS) formulation is appropriate, see [1, 6]. Here we seek minimal corrections G to B and E to A giving a compatible corrected system,

$$\min_{G,E,X} \|[G,E]\|_F \quad \text{subject to} \quad (A+E)X = B+G.$$

While the solvability analysis of the ordinary least squares method (LS) is straightforward, this is not the case for the TLS analyzed in full generality recently in [3]. In this talk, we summarize the latest solvability results on selected least squares methods for problems with multiple observations. We discuss also the core reduction [5, 4, 2] allowing to remove all irrelevant or redundant data from the original approximation problem.
When the observations correspond to some parameters independent of the model A, it can be advantageous to organize the columns of B into a tensor $\mathcal{B}$ reflecting the structure

of the parameter sampling. Then the original approximating problem takes the form

$$A \times_1 \mathcal{X} \approx \mathcal{B}, \quad \mathcal{X} \in \mathbb{R}^{n \times d_2 \times \ldots \times d_k}, \mathcal{B} \in \mathbb{R}^{m \times d_2 \times \ldots \times d_k}.$$

While the LS has already been generalized to such multilinear problems, this is to our knowledge not the case for the TLS. In this contribution, we propose possible tensor TLS definition and investigate its properties including relation to the linear TLS formulation above.

[1] Golub, G. H., Van Loan, C. F.: An analysis of the total least squares problem. Numer. Anal. **17** (1980), pp. 883–893.

[2] Hnětynková, I., Plešinger, M., Sima, D. M.: Solvability of the core problem with multiple right-hand sides in the TLS sense. SIAM J. on Matrix Anal. and Appl. **37** (2016), pp. 861–876.

[3] Hnětynková, I., Plešinger, M., Sima, D. M., Strakoš, Z., Van Huffel, S.: The total least squares problem in $AX \approx B$. A new classification with the relationship to the classical works. SIAM J. Matrix Anal. Appl. **32** (2011), pp. 748–770.

[4] Hnětynková, I., Plešinger, M., Strakoš, Z.: The core problem within a linear approximation problem $AX \approx B$ with multiple right-hand sides. SIAM J. Matrix Anal. Appl. **34** (2013), pp. 917–931.

[5] Paige, C. C., Strakoš, Z.: Core problem in linear algebraic systems. SIAM J. Matrix Anal. Appl. **27** (2006), pp. 861–875.

[6] Van Huffel, S., Vandewalle, J.: The Total Least Squares Problem: Computational Aspects and Analysis. SIAM Publications, Philadelphia, PA, 1991.

Nonnegative matrix factorization through sparse regression

R. Luce 14:40

We consider the problem of computing a *nonnegative low rank factorization* to a given nonnegative input matrix under the so-called "separability condition". This assumption makes this otherwise NP hard problem polynomial time solvable, and we will use first order optimization techniques to compute such a factorization. The optimization model use is based on sparse regression with a self-dictionary, in which the low rank constraint is relaxed to the minimization of an $\ell_1$1-norm objective function. We apply these techniques to endmember detection and classification in hyperspectral imaging data.

Parametrized Sylvester Equations in Model Order Reduction

M. Hund (Max Planck Institute for Dynamics of Complex Technical Systems), J. Saak (Max Planck Institute for Dynamics of Complex Technical Systems) 15:00

Sylvester equations of the form

$$AV\tilde{E} + EV\tilde{A} = BL \tag{6.12}$$

are a key player in model order reduction (MOR) of linear input-output systems as

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t), \end{aligned}$$

with a regular matrix $E \in \mathbb{R}^{n\times n}$, as well as matrices $A \in \mathbb{R}^{n\times n}, B \in \mathbb{R}^{n\times p}, C \in \mathbb{R}^{q\times n}$ and $\tilde{A}, \tilde{E} \in \mathbb{R}^{m\times m}$, where $m \ll n$.
These arise in the context of the $\mathcal{H}_2$ optimality conditions of Wilson [5], the variation [2] of the orthogonal polynomial time domain MOR framework in [3], as well as in classical moment matching [4].
There are different ways parametrized Sylvester equations may arise in MOR. On the one hand, in the time domain approach, one ends up with a Sylvester equation (6.12), where $\tilde{A}$ is the identity $I_m \in \mathbb{R}^{m\times m}$. The solution of this Sylvester equation spans the same Krylov subspace as moment matching with the generalized eigenvalues of $(I_m, \tilde{E})$ as expansion points. Now, when using parametrized families of Jacobi polynomials a Sylvester equation

$$AV\tilde{E}(\mu) + EV = BL$$

arises that is parametrized with $\mu \in \mathbb{R}^2$ in the small matrix $\tilde{E}(\mu)$.
On the other hand, considering parametrized dynamical systems

$$\begin{aligned} E(\mu)\dot{x}(t) &= A(\mu)x(t) + B(\mu)u(t), \\ y(t) &= C(\mu)x(t), \end{aligned}$$

with parameter $\mu \in \mathbb{R}^d$, provides a Sylvester equation that is now parametrized in its large, but sparse matrices

$$A(\mu)V\tilde{E} + E(\mu)V\tilde{A} = B(\mu)L.$$

Our final goal is to solve the $\mathcal{H}_2$ optimal MOR problem via a fixed point iteration on the Wilson conditions along the lines of the two sided iterative approximation (TSIA) algorithm. This could in turn serve as an alternative parametrized $\mathcal{H}_2$ optimal MOR algorithm to the "parametric IRKA" [1]. In our contribution, we will present first results towards this goal.

[1] U. Baur, C. A. Beattie, P. Benner, and S. Gugercin, *Interpolatory projection methods for parameterized model reduction*, SIAM J. Sci. Comput., 33 (2011), pp. 2489–2518.

[2] M. Hund and J. Saak, *A connection between time domain model order reduction and moment matching*, Proc. Appl. Math. Mech., 16 (2016).

[3] Y.-L. Jiang and H.-B. Chen, *Time domain model order reduction of general orthogonal polynomials for linear input-output systems*, IEEE Trans. Automat. Control, 57 (2012), pp. 330–343.

[4] A. Vandendorpe, *Model reduction of linear systems, an interpolation point of view*, PhD thesis, Université Catholique De Louvain, 2004.

[5] D. A. Wilson, *Optimum solution of model-reduction problem*, in Proceedings of the Institution of Electrical Engineers, 1970, pp. 1161–1165.

Dimension reduction approach to the parameter dependent quadratic eigenvalue problem

Z. Tomljanović (University of Osijek), N. Truhar (University of Osijek) 15:20

We consider the quadratic eigenvalue problem given by

$$(\lambda^2(\mathbf{v})M + \lambda(\mathbf{v})D(\mathbf{v}) + K)x(\mathbf{v}) = 0,$$

where M, K are positive definite Hermitian $n\times n$ matrices and $D(\mathbf{v})$ is an $n\times n$ Hermitian semidefinite matrix which depends on a parameter vector $\mathbf{v} = \begin{bmatrix} v_1 & \dots & v_k \end{bmatrix} \in \mathbb{R}^k_+$.
We will present some results on eigenvalue and eigensubspace behavior, which depend on the structure of the considered quadratic eigenvalue problem.
In particular, we will show results on the efficient calculation of all or just one important part of the eigenvalues of the parameter dependent quadratic eigenvalue problem, for a different sets of parameters $\mathbf{v}$. With the new approach one can efficiently (and accurately enough) calculate all (or just one part of the) eigenvalues even for the case when v_i are of the modest magnitude. Moreover, for both cases of approximations, we have derived the corresponding upper error bounds.
The new approximations and upper bound allow us to track the movements of eigenvalues in the complex plane depending on the parameter $\mathbf{v}$.

Adaptive FETI-DP and BDDC Methods with a Transformation of Basis

M. Kühn, A. Klawonn (Mathematical Institute, University of Cologne), O. Rheinbach (Institute of Numerical Mathematics and Optimization, TU Freiberg) 15:40

Adaptive Coarse Spaces for the FETI-DP (Finite Element Tearing and Interconnecting) and BDDC (Balancing Domain Decomposition by Constraints) domain decomposition methods are considered. These adaptive coarse spaces are based on the computation of small local eigenvalue problems. A special emphasis is put on the three dimensional case and on materials with heterogeneous material parameters where coefficient jumps are not aligned with the interface of the domain decomposition. Our new approach is based on solving local eigenvalue problems on faces, enriched by a selected, small number of additional local eigenvalue problems on edges. The additional edge eigenvalue problems make the method provably more robust. The introduction of the additional

edge eigenvalue problems yields a condition number that only depends on the tolerance of the local eigenvalue problems and some properties of the domain decomposition and is independent of discontinuities of the material parameters. Until recently, we have implemented the adaptive constraints by a balancing (or deflation) approach. In the present work, we use a transformation of basis approach in combination with partial subassembly. Compared to the case of constant coefficients on subdomains, the transformation of basis approach has to be adapted for general heterogeneous materials. Numerical results are shown for linear elasticity and composite materials supporting our theoretical findings.

S 17 : Applied and numerical linear algebra

Tuesday 16:30 - 18:30 Coudraystr. 11C, Room 202

Structured randomized low-rank algorithms

D. Kressner (EPFL) 16:30

The randomized SVD is an effective and simple way to obtain a low-rank approximation of a large matrix A, and it proceeds by multiplying A with a few random vectors. In this talk, we discuss the benefits of imposing further structure on these random vectors. Specficially, we discuss the case where each vector is the outer product of two small random vectors. Depending on the application, this may considerably reduce the effort of multiplying with A. We explain that this is the case in the recompression of certain tensors and various tasks associated with matrix functions. This talk is based on joint work with Lana Perisa and Zvonimir Bujanovic.

Bootstrap AMG for tensor structured Markov chains

S. Sokolovic (Bergische Universität Wuppertal (BUW)) 17:10

We want to compute the stationary distribution of a tensor structured continuous time Markov chain (CTMC), which leads to a singular linear system of the form $Ax = 0$ with

$$A = \sum_{(s,t)} \bigotimes_i E_i^{(s,t)} - \sum_{(s,t)\neq(i,i)} \bigotimes_i D_i^{(s,t)} \in \mathbb{R}^{\prod n_i \times \prod n_i}.$$

There, the size of the so-called generator matrix A can easily explode, which is known as the *curse of dimensionality*. Tensorized techniques in iterative methods for solving this task are therefore necessary.
In this talk we investigate a tensorized version of the bootstrap algebraic multigrid framework. The bootstrap method has the nice feature—amongst others—to adaptively construct the interpolation operator by a least squares approach. In this talk we show that the task to adapt this method to a tensor setting is not straightforward and that it turns out that the most difficult part is to find reasonable test vectors for the least squares interpolation.

The efficiency of the tensorized bootstrap method will be shown in some numerical tests from different application areas.

The Geometrical Description of Feasible Singular Values in the Tensor Train Format

S. Kraemer (RWTH Aachen University) 17:30

Tensors have grown in importance and are applied to an increasing number of fields. Crucial in this regard are tensor formats, such as the widespread Tensor Train (TT) decomposition, which represent low rank tensors. This multivariate TT-rank and accordant $(d-1)$-tuples of singular values are based on different matricizations of the same d-dimensional tensor. While the behavior of these singular values is as essential as in the matrix case ($d = 2$), here the question about the *feasibility* of specific TT-singular values arises: for which prescribed tuples exist correspondent tensors and how is the topology of this set of feasible values?
This work is largely based on a connection that we establish to eigenvalues of sums of hermitian matrices. After extensive work spanning several centuries, that problem, known for Horn's conjecture, was basically solved by Knutson and Tao through the concept of so called *honeycombs*. We transfer and expand their and earlier results on that topic and thereby find that the set of feasible TT-singular values is geometrically described by polyhedral cones, resolving our problem setting to the largest extend. Besides analytical results, we also present a linear programming algorithm to check feasibility as well as a simple heuristic, but reliable algorithm to construct tensors with prescribed, feasible singular values.

Tensor Representation of Many-Particle Potentials

V. Khoromskaya (Max-Planck-Institute for Mathematics) 17:50

Rank-structured tensor approach appeared to be efficient for the numerical treatment of the long-range electrostatic potentials in many-particle systems, like small crystalline clusters, and biomolecules, where the summation of the electrostatic potentials in large finite volumes is one of the challenging problems. The basics of the method is the canonical tensor representation of a single Newton kernel defined on fine $n \times n \times n$ 3D Cartesian grids, which was first used for accurate calculation of the integral operators in the Hartree-Fock equation [3].
Summation of the long-range potentials on $L \times L \times L$ 3D lattices is reduced to assembling of the vectors of the side matrices in the canonical/Tucker tensors [2], yielding computational complexity of the order of $O(L)$ which is much less compared with $O(L^3)$ in traditional approaches, like Ewald-type summation. The canonical tensor rank of the resulting sum of a large number of potentials positioned on rectangular 3D lattices is the same as for tensor representation of a single Newton kernel. For lattices with multiple vacancies the rank is increased by a small factor.
Recently introduced Range-Separated (RS) tensor format [1] applies to arbitrarily located potentials. It splits the grid-based tensor representation of the electrostatic

potentials into long- and short-range parts. Then the canonical rank of the long-range part of the sum computed by the reduced higher order SVD [3] only logarithmically depends on the number of particles in the multiparticle system. While the short-range contributions are of local character and do not effect the particles around. The numerical examples for protein-type systems are presented.

[1] P. Benner, V. Khoromskaia and B. N. Khoromskij. *Tensor Summation of Many-particle Potentials*. Preprint arXiv:1606.09218, 2016.
[2] V. Khoromskaia, B.N. Khoromskij. *Grid-based Lattice Summation of Electrostatic Potentials by Assembled Rank-structured Tensor Approximation.* CPC, 185 (2014), pp. 3162-3174.
[3] B. N. Khoromskij and V. Khoromskaia. *Multigrid Tensor Approximation of Function Related Arrays.* SIAM J Sci. Comp., **31**(4), 3002-3026 (2009).

Numerical Methods for Delamination and DCB Test Problems

N. Ovcharova (Universität der Bundeswehr München) 18:10

We present several efficient numerical methods for nonsmooth problems in nonmono tone contact mechanics. Examples include adhesive contact problems, delamination and crack propagation in DCB tests. A challenging problem is adhesive bonding in case of contamination. The nonsmoothness comes from the nonsmooth data of the problems itself, in particular from nonmonotone, multivalued physical laws involved in the boundary conditions. The variational formulation of the resulting boundary value problems leads to a class of nonsmooth variational inequalities. The resulting variational inequality problem is first regularized and then discretized by either finite element or boundary element methods. In addition, we propose a novel regularized mixed formulation and provide a reliable a-posteriori error estimate enabling also hp-adaptivity. Another approach to solve the nonsmooth variational problem is by the strategy: first discretize by finite elements, then optimize using finite dimensional nons mooth optimization methods. We propose a new bundle method for solving nonconvex optimization problems that has been successfully used to simulate the process of delamination in composite materials. Various numerical experiments illustrate the behavior, the strength and the weaknesses of the proposed approximation schemes. Finally, we demonstrate the applicability of those methods in numerical simulation of DCB test problems.

S 17 : Applied and numerical linear algebra

Wednesday 14:00 - 16:00 Coudraystr. 11C, Room 202

Counting Fiedler pencils with diagrams

F. Poloni (University of Pisa), G. Del Corso (University of Pisa) 14:00

Fiedler pencils (with repetitions) are a family of matrix pencils which generalizes the well-known companion form: they are \emph{linearizations} of matrix polynomials, i.e., they provide a template to construct, given a matrix polynomial, a linear eigenvalue problem with the same eigenvalues and multiplicity.
Fiedler pencils are constructed as product of special block matrices that act nontrivially only on two contiguous blocks. They have a rich structure that gives rise to many combinatorial properties.
In this talk, we introduce a notation that associates to each pencil a diagram that depicts its action on the blocks. Using this notation, we can obtain visual proofs of several statements in the theory, and we can solve several counting problems (such as "how many distinct Fiedler pencils with repetitions of a given dimension exist"). Among them, in particular, we are interested in counting Fiedler pencils associated to symmetric and palindromic matrix polynomials which preserve the same structure.

A new structure-preserving first order formulation for polynomial eigenvalue problems

M. Froidevaux (TU Berlin), D. Kressner (EPFL), V. Mehrmann (TU Berlin) 14:40

In this talk we consider polynomial eigenvalue problems (EVPs) $\lambda^k A_k v + \cdots + \lambda A_1 v + A_0 v = 0$, where $A_k, \ldots, A_0$ are rectangular matrices. In practice, when the eigenvalue problem arises from the discretization of a physical system, the matrix polynomial often has a particular structure (e.g. Hermitian, odd, even, palindromic), which implies a symmetry in the spectrum. The most common approach in the resolution of polynomial EVPs is to proceed via linearization. However, usual linearizations destroy the structure of the problem and, when the matrix polynomial is singular, elongate some of the singular chains. This can lead to a loss of efficiency and accuracy in the computed results. In this talk, we will introduce a new structure-preserving first order formulation for polynomial EVPs, and to avoid technical complexity, will focus on the quadratic case. We will present a complete algorithm for the computation of eigenvalues in structured and in general quadratic EVPs, as well as show numerical comparisons with the MATLAB function `polyeig` and with the implementation of the `quadeig` algorithm [1].

[1] S. Hammarling, C. J. Munro, and F. Tisseur. An algorithm for the complete solution of quadratic eigenvalue problems. ACM Transactions on Mathematical Software, 39(3):18:1–18:19, 2013.

The symmetric eigenvalue problem by edge elimination in a hypergraph

K. Kahl (Bergische Universität Wuppertal) 15:00

In this talk we show that the calculation of all eigenvectors and eigenvalues of a symmetric (sparse) matrix can be expressed by subsequently eliminating all edges in a hypergraph associated to the matrix. The elimination of each edge requires the calculations of all solutions of a secular equation, where the number of solutions is equal to the number of nodes in the removed hyperedge.
The approach allows to study the symmetric eigenvalue problem in a spirit similar to Gaussian elimination, which in essence is simply a successive node elimination algorithm. Just as with Gaussian elimination, where a symbolic phase can be carried out before the actual calculation to reduce the fill-in in the matrix during the elimination, one can to try to find an edge elimination ordering that minimizes the total number of solutions in the secular equations over the whole elimination process.
We wrap up the talk with a few observations and remarks on the algorithm with respect to complexity bounds, intermediate quantities and connections to other existing algorithms and show some results on heuristics to find optimal elimination strategies, largely motivated by approaches used in Gaussian elimination (e.g., minimum degree).

Generalizing diffuse interface methods on graphs: non-smooth potentials and hypergraphs

M. Stoll (MPI Magdeburg) 15:20

Diffuse interface methods have recently been introduced for the task of semi-supervised learning. The underlying model is well-known in materials science but was extended to graphs using a Ginzburg–Landau functional and the graph Laplacian. We generalize the previously proposed model by a non-smooth potential function. Additionally, we show that the diffuse interface method can be used for the segmentation of data coming from hypergraphs. For this we show that the graph Laplacian in almost all cases is derived from hypergraph information. Additionally, we show that the formerly introduced hypergraph Laplacian coming from a relaxed optimization problem is well suited to be used within the diffuse interface method. We present computational experiments for graph and hypergraph Laplacians.

The Radau–Lanczos method for matrix functions

M. Schweitzer (Bergische Universität Wuppertal) 15:40

When using Krylov subspace methods for approximating $f(A)\mathbf{b}$, the action of a matrix function on a vector, the number of iterations that can be performed is often limited by the available memory, as one needs to store the whole Krylov basis even for Hermitian A. To overcome these limitations, several implementations of restarted Krylov subspace methods for matrix function computations have been proposed and analyzed in the literature in recent years. While these methods are often very successful, and convergence of the restarted methods can be guaranteed for large classes of functions and matrices, the speed of convergence can be very slow for small restart lengths. Therefore, for

large scale problems or in other situations where memory is very scarce, acceleration techniques for improving the speed of convergence are of high interest.
We present one such acceleration technique which is based on a rank-one update of the tridiagonal Lanczos matrix, motivated by the connection between the Lanczos process and Gauss–Radau quadrature. We prove that the modified method is still guaranteed to converge to $f(A)\mathbf{b}$ when A is Hermitian positive definite and f is a Stieltjes function, and motivate why the new method can be expected to improve over the standard restarted Lanczos method in many cases. This is confirmed in numerical experiments involving real-world applications.

S 17 : Applied and numerical linear algebra

Wednesday 16:30 - 18:30 Coudraystr. 11C, Room 202

Iterative Solvers for Helmholtz Problems: AILU Factorizations, Sweeping Preconditioners, Source Transfer, Single Layer Potentials, Polarized Traces, and Optimal and Optimized Schwarz Methods

M. Gander (University of Geneva) 16:30

I explain in my presentation the underlying mathematical structure of the many recently developed iterative Helmholtz solvers mentioned in the title. I will show that at the discrete level, they are all based on the approximation of an exact block LU factorization, and at the continuous level, they are all approximations of an optimal Schwarz method. This relation reveals that while these methods have a certain potential, there are also important limitations for these methods. The results I present are joint work with Hui Zhang.

Multigrid smoothers for the Stokes problem

L. Claus (Universität Kassel), M. Bolten (Universität Kassel) 17:10

Multigrid methods are efficient iterative solvers for the solution of partial differential equations (PDEs). The efficiency of multigrid methods is due to the combination of suitable smoothers with a coarse grid correction. As one of the two key ingredients smoothers have a significant impact on the performance of multigrid solvers.
Most of the literature on smoothers in multigrid methods is concerned with scalar PDEs, only. Systems are considered less often.
In this talk, we present a comparative study of several smoothers for multigrid methods for the solution of the Stokes equations. Besides the commonly used Vanka smoother and the Braess-Sarazin smoother, we also consider a non-overlapping variant of the Vanka smoother. While the latter is computationally cheaper, the convergence depends much more on the implementation than that of the overlapping method. We consider discretization using appropriate finite elements as well as by finite differences on staggered

grids. A comparison including the computational cost and the convergence properties of the different methods will be presented.

Preconditioned GMRES Revisited

R. Herzog (TU Chemnitz), K. Soodhalter (Johann Radon Institute for Computational and Applied Mathematics (RICAM)) 17:30

The generalized minimal residual method (GMRES) introduced by Saad and Schultz in 1986 is one of the most popular iterative solvers for general linear systems $A\,x = b$. Interestingly, there does not seem to be a consensus in the literature on the definition of *preconditioned* GMRES.
We shed some light on this issue from the point of view of linear systems in Hilbert spaces. We compare various common implementations of preconditioned GMRES with respect to their convergence analysis and practical performance.

Fourier Analysis of Periodic Stencils in Multigrid Methods

H. Rittich (Bergische Universität Wuppertal) 17:50

Many applications require the solution of a partial differential equations. A discretization these equations often leads to large and sparse linear systems. In many situations a multigrid method can solve these systems efficiently. To adapt a multigrid method to a given problem, Local Fourier Analysis (LFA) can be used. It makes quantitative predictions about the behavior of the components of a multigrid methods.
We present a formulation of LFA for multigrid methods which involve periodic stencils. We discuss how periodic stencils can be used to construct an idealized formulation of certain multigrid methods. Furthermore, we show how this formulation can be used to automate LFA via software.

Block Krylov subspace methods for computing functions of matrices applied to multiple vectors

K. Lund (Bergische Universität Wuppertal (BUW)), A. Frommer (Bergische Universität Wuppertal (BUW)), D. Szyld (Temple University) 18:10

Since Dianne O'Leary's seminal paper on block conjugate gradients (CG) in 1980, block Krylov subspace methods have been used widely to solve linear systems with multiple right-hand sides. Recently, these methods have been used to compute $f(A)B$, where f is a scalar function defined on the matrix $A \in \mathbb{C}^{n\times n}$ and $B \in \mathbb{C}^{n\times s}$. Hinging on a generalized framework for block Krylov subspaces that encompasses established results not only for the "classical" block methods (as in O'Leary's work), but also for global methods and the newer "loop-interchange" methods, we develop a detailed theory for block Krylov methods for $f(A)B$.
This framework rests on the choice of a subalgebra $\mathbb{S} \subset \mathbb{C}^{s\times s}$ and a block inner product $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ mapping from $\mathbb{C}^{n\times s} \times \mathbb{C}^{n\times s}$ onto $\mathbb{S}$. Pairing $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ with a scaling quotient N leads to block notions of orthogonality and normalization and consequently a generalization of the block Arnoldi procedure. From all this, we define a block full orthogonalization

method for functions of matrices (B(FOM)^2) whose approximations lie in a generalized block Krylov subspace.
The B(FOM)^2 approximation is not without shortcomings. Memory restrictions may prevent one from storing enough basis vectors to compute an accurate solution. Therefore, we also incorporate restarts, based on an efficient update formula for the error, which is itself a matrix function applied to multiple vectors.
We show that the restarted B(FOM)^2 converges with a CG-like bound for Hermitian positive definite matrices A and Stieltjes functions f. Our convergence results hold not only for the classical, global, and loop-interchange methods but also for any appropriate combinations of $\mathbb{S}$, $\langle\!\langle \cdot, \cdot \rangle\!\rangle$, and N. Such generality opens the door for other methods that could lead to further computational improvements.
We demonstrate the performance and versatility of different versions of the B(FOM)^2 in a variety of numerical experiments, even for non-Hermitian matrices and non-Stieltjes functions. The global version of B(FOM)^2 performs excellently in comparison to the classical and loop-interchange versions, and especially in comparison to the non-block method of computing each column of $f(A)B$ separately.

S 17 : Applied and numerical linear algebra

Thursday 14:00 - 16:00 Marienstr. 7, 1st floor, Room 102

Bounds for the off-diagonal decay in inverses and Cauchy–Stieltjes functions of banded, normal matrices based on complex Chebyshev polynomials

C. Schimmel (Bergische Universität Wuppertal (BUW)) 14:00

It is known that in many functions of banded Hermitian positive definite matrices, the entries exhibit a rapid decay away from the main diagonal. This is in particular true for the inverse, and based on results for the inverse, bounds for Cauchy–Stieltjes functions of Hermitian positive definite matrices have recently been obtained. We add to the known results by considering the more general case of normal matrices, for which fewer practically relevant results exist. Starting from a very general estimate based on approximation properties of Chebyshev polynomials on ellipses, we obtain as special cases insightful decay bounds for various classes of normal matrices, including (shifted) skew-Hermitian and Hermitian indefinite matrices. In addition, some of our results improve over known bounds when applied to the Hermitian positive definite case.

A Greedy Subspace Method for Computing the H-infinity-Norm

N. Aliyev (Koc University), P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems), E. Mengi (Koc University), M. Voigt (Technische Universität Berlin) 14:20

In this talk we consider functions of the form

$$G(s) = C(s)D(s)^{-1}B(s),$$

where $B(\cdot)$, $C(\cdot)$, and $D(\cdot)$ are matrix-valued functions meromorphic in the open right complex half-plane. Transfer functions of linear, but also many nonlinear systems (such as delay systems) can be put into this framework.
In this contribution we consider $\mathcal{H}_\infty$-functions $G(\cdot)$ (i. e., functions which are analytic and bounded in the open right complex half-plane) and discuss the computation of their $\mathcal{H}_\infty$-norm, namely

$$\|G\|_{\mathcal{H}_\infty} := \sup_{\omega\in\mathbb{R}} \|G(\mathrm{i}\omega)\|_2 .$$

This norm is essential in many applications of robust control and model order reduction of dynamical systems. We focus on the case where the size of $D(\cdot)$ is very large compared to the number of rows of $C(\cdot)$ and the number of columns of $B(\cdot)$. We propose a subspace projection method to obtain approximations of $G(\cdot)$ by interpolation techniques. The norm values are computed for the resulting reduced functions, then the subspaces are refined by means of the optimal points on the imaginary axis where the maximum singular value of the reduced function is attained. The subspace method is designed so that certain Hermite interpolation properties hold between the largest singular values of the original and reduced functions. This leads to a superlinearly convergent algorithm with respect to the subspace dimension, which we prove and illustrate on various numerical examples.

[1] N. Aliyev, P. Benner, E. Mengi, and M. Voigt. Large-scale computations of $\mathcal{H}_\infty$-norms by a greedy subspace method, July 2016. Submitted for publication.

The dynamical impact of structural perturbations in electrical circuits

J. Pade (HU Berlin), C. Tischendorf (HU Berlin) 14:40

The function of many electrical circuits is defined through the stability of a fixed point. Assume that due to damage or other external influences the value of a circuit's element is perturbed. Even the simplest example shows that determining whether such a structural perturbation has a stabilizing or a destabilizing effect in terms of the circuit's topology is very hard. The underlying algebraic problem is given by a spectral analysis of an associated (Laplacian) matrix pencil. In particular, we are interested in the direction of motion of its spectral gap under the above perturbations. While the spectrum of Laplacian matrices is well investigated and much is known about its connection to the structure of the underlying graph, the situation is more involved for matrix pencils. Here we present first perturbation results with applications to electrical circuits.

OS-ACMS: A Multiscale Coarse Space For Overlapping Schwarz Methods Based On The ACMS Space In Two Dimensions

J. Knepper, A. Heinlein (Mathematical Institute, University of Cologne), A. Klawonn (Mathematical Institute, University of Cologne), O. Rheinbach (Institute of Numerical Mathematics and Optimization, TU Freiberg) 15:00

Robust domain decomposition methods for solving second order elliptic problems with large variations in the coefficient rely on the construction of a suitable coarse space. We propose two-level overlapping Schwarz methods using coarse spaces constructed from the Approximate Component Mode Synthesis (ACMS) multiscale discretization. In particular, we make use of eigenvalue problems using local Schur complements on subdomain edges. The convergence of a corresponding preconditioned Krylov method depends only on a user-specified tolerance and is therefore independent of variations of the coefficient function. The proposed methods also benefit from the low dimension of the local eigenvalue problems and from the fact that they can be solved approximately at the cost of only one or two iterations of LobPCG.

S 18: Numerical methods of differential equations

Organizers: Rolf Krause (USI - Università della Svizzera italiana)
Gerhard Starke (Universität Duisburg-Essen)

S 18 : Numerical methods of differential equations

Thursday 14:00 - 16:00 Coudraystr. 11C, Room 202

Space-Time Isogeometric Analysis of Parabolic Initial-Boundary Value Problems

U. Langer (Johannes Kepler University Linz) 14:00

We look at parabolic initial-boundary value problems from an elliptic point of view treating the time derivative as a convection term in time. More precisely, we propose stable space-time IgA variational schemes, the mesh-dependent bilinear form of which is uniformly elliptic on the IgA space with respect to a special mesh-dependent norm. This ellipticity property together with a corresponding boundedness result, consistency and approximation results for the IgA spaces yields convergence rate estimates in the mesh-dependent norm. In contrast to implicit time-stepping methods, we have to solve only one huge system of linear algebraic equations. This can very efficiently be done by algebraic or special geometric multigrid methods on parallel computers. We also present functional a posteriori error estimates that can be used for devising adaptive schemes. The talk is based on joint papers with Svetlana Matculevich, Stephen Moore, Martin Neumüller, Sergey Repin and Ioannis Toulopoulos.

The author would like to thank the Austrian Science Fund (FWF) for the financial support under the grants S 117-03.

Space-Time Boundary Integral Equations of the Time Fractional Diffusion Equation

S. Bonkhoff (Technische Universität Graz) 14:20

In this talk we consider initial boundary value problems of the time fractional diffusion equation in a space-time cylinder with a time derivative of order $\alpha \in (0, 1)$. This fractional differential equation arises in mathematical modeling of anomalous sub-diffusion processes, where the time fractional derivative replaces the first order time derivative of the standard diffusion equation. For this purpose we investigate two definitions of fractional derivatives, the Riemann-Liouville definition and the Caputo one.
As a starting point of the numerical investigation we construct a fundamental solution of the time fractional diffusion equation by means of the Fox H-functions and represent the solution in terms of layer potentials. With this approach we derive appropriate boundary integral equations and investigate the behaviour of the layer potentials in anisotroptic Sobolev spaces.

Space-Time Boundary Integral Equations and an Adaptive Boundary Element Method for the Wave Equation

M. Zank (TU Graz) 14:40

For the discretisation of the wave equation by boundary element methods the starting point is the so-called Kirchhoff's formula, which is a representation formula by means of boundary potentials. In this talk different approaches to derive weak formulations of related boundary integral equations are considered. First, a brief overview of the Laplace transform method with boundedness and coercivity estimates in appropriate Sobolev spaces is given. Second, a space-time energetic formulation is motivated and discussed. For this space-time energetic formulation a space-time boundary element method is introduced and to derive an adaptive scheme an a posteriori error estimator based on the representation formula is used.
Finally, numerical examples for a one-dimensional spatial domain are presented and discussed.

Time Domain BEM Based on Generalised Convolution Quadrature

H. Diao (Universität Zürich) 15:00

In this talk we present the application of the *generalised convolution quadrature* (gCQ) technique to the time domain boundary element method (BEM) which solves the retarded potential boundary integral equation (RPBIE). Our result allows to employ the multi-stage Runge-Kutta method as the time stepping scheme for the generalised convolution quadrature which is used in the time domain BEM for acoustic problems in either a bounded three-dimensional domain or in its unbounded exterior.

As a model problem, we consider the three-dimensional wave equation with impedance boundary condition. The application of either single layer potential or double layer potential to the time-dependent boundary condition leads to a convolution whose kernel function comprises the boundary integral operators. We use gCQ for the temporal discretisation and Galerkin BEM for the spatial discretisation, which results in a linear block system to be solved at each time step.
This technique can also be applied to other boundary conditions as well as to different formulations of boundary integral equations.

Time domain boundary elements for screen and contact problems

F. Meyer (University of Stuttgart), H. Gimperlein (Heriot-Watt University), E. Stephan (Leibniz University Hannover), C. Oezdemir (Leibniz University Hannover) 15:20

Due to their robustness and efficiency boundary element methods are a frequently used tool for the approximate numerical solution of partial differential equations in many areas of engineering and science. We discuss time domain boundary element methods for the scalar wave equation, especially for singular geometries and nonlinear contact boundary conditions which play an important role in numerous applications in mechanics.

First we consider edge and corner singularities for the wave equation. Time independent a priori graded meshes lead to efficient approximations as confirmed by numerical experiments for wave scattering from screens. We further consider a dynamic contact problem with flat contact area, which corresponds to a variational inequality for the Dirichlet-Neumann operator for the wave equation. We present well-posedness as well as a priori error estimates for a time domain Galerkin boundary element method. The dynamic contact problem is solved by an efficient time stepping scheme for which we present some numerical experiments on uniform meshes.

A space-time FEM for elastic bars with application to dynamic truss analysis

A. Meeh (Technische Universität Graz), M. Gfrerer, D. Pölz, M. Schanz 15:40

We propose a space-time FEM (finite element method) for the dynamic bar problem and apply it to analyze truss systems. The bar problem is governed by the scalar wave equation supplemented by initial and boundary conditions. The idea is to solve this problem with a space-time FEM using unstructured meshes in the space-time domain. We derive a variational formulation by weighting the governing equation with the time derivative of test functions and apply integration by parts to the spatial derivative. Existing formulations are based on reformulation of the governing equation into a first order system (see e.g. [1] and the references therein). In contrast to these formulations, our approach uses only the primal variable, the extension of the bar. Due to the second time derivative in the inertia term classical C^0 elements are not appropriate. In a similar way this problem arises in thin plate bending, where C^1 elements are needed. In order to allow for a simple adaptive discretization, we use a triangulation of the space-time

domain. A well known triangular C^1 element is the Argyris element, which we use for the discretization. The Argyris element is of Hermite type and spans the full space of bivariate polynomials of degree five. Our implementation of the Argyris element is based on [2]. We verify our approach by evaluating the order of convergence for the L_2 error. Finally, we apply the developed FEM to a truss system.

[1] Anderson, M. and Kimn, J.-H., *A numerical approach to space-time finite elements for the wave equation.* Journal of Computational Physics 226.1 (2007): 466-476

[2] Domínguez, V. and Sayas, F-J., *Algorithm 884: A simple Matlab implementation of the Argyris element.* ACM Transactions on Mathematical Software 35.2 (2008): 16.

S 18 : Numerical methods of differential equations

Thursday 16:30 - 18:30 Coudraystr. 11C, Room 202

A reliable, efficient and localized error estimator for a discontinuous Galerkin method for the Signorini problem.

M. Walloth (Technische Universität Darmstadt) 16:30

An adaptation of the finite element mesh by means of a posteriori error estimators is indispensable for an efficient and accurate numerical simulation of contact problems. We present a new reliable and efficient residual-type a posteriori error estimator for the discontinuous finite element solution of contact problems. Numerical examples confirm our theoretical results.
The theoretical results are derived for two and three-dimensional domains and arbitrary gap functions. Exemplary, we deal with the symmetric interior penalty method. It will turn out that in the case no actual contact occurs, the new error estimator coincides with the standard residual error estimator for linear elliptic problems. The estimator yields upper and lower bounds to a suitable error norm which measures the error in the displacements and in a quantity related to the contact stresses and the actual contact zone. In the derivation of the error estimator the so-called Galerkin functional, replacing the role of the linear residuals, plays an important role. In [1] the approach was used for continuous finite elements. The local properties of the discontinuous solution are exploited appropriately so that, on the one hand, the error estimator has no contributions related to the non-linearity in the so-called full-contact zone and, on the other hand, the critical region between the actual and non-actual contact zone can be well refined. We like to emphasize that due to the right splitting of the contributions of the Galerkin functional we can exploit cancellation properties. Compared to the case of continuous finite elements for contact problems [1] the definition of full-contact is more localized.

[1] R. Krause, A. Veeser, M. Walloth, An efficient and reliable residual-type a posteriori error estimator for the Signorini problem, Numer. Math. 130 (1) 2015, pp.151-197.

Stress reconstruction for the nonconforming P2 finite element method and a posteriori error estimation

M. Moldenhauer (University Duisburg-Essen), G. Starke (University Duisburg-Essen) 16:50

Stress reconstruction for the nonconforming P2 finite element method and a posteriori error estimation

Marcel Moldenhauer[‡], Gerhard Starke[†]

We want to follow the framework given in [1] and present an a posteriori error estimator for the nonconforming P2 finite element method of the linear elasticity problem based on a nonsymmetric H(div)-conforming approximation of the stress tensor.
In [2] a nonconforming P2 finite element method was used with success to reconstruct an H(div)-conforming flux with application to a posteriori error estimation. We want to study the positive characteristics of nonconforming P2 elements in the framework of [1] and confirm the quality of our stress reconstruction and effectiveness of our error estimator with numerical examination of the Cooks membran problem. See also [3].

[1] Kwang-Yeon Kim, A posteriori error estimator for linear elasticity based on nonsymmetric stress tensor approximation, *J. KSIAM Vol.16, No.1, 1-13, 2011*

[2] Kwang-Yeon Kim, Flux reconstrucion for the P2 nonconforming finite element method with application to a posteriori error estimation, *Applied Numerical Mathematics 62 (2012) 1701-1717*

[3] B. Müller, G. Starke, Stress-based Finite Element Methods in Linear and Nonlinear Solid Mechanics, Advanced Finite Element Technologies, CISM International Centre for Mechanical Sciences vol.566, p. 69-104, Stringer 2016, J. Schröder and P. Wriggers

Stress-based mixed finite elements for elasticity

F. Bertrand (Universität Duisburg-Essen), G. Starke (Universität Duisburg-Essen), M. Moldenhauer (Universität Duisburg-Essen) 17:10

Computations in solid mechanics are usually performed using the displacements as primal variable. As accurate stress approximations are of interest in many applications in solid mechanics, their reconstruction has to be produced carefully. In particular, reconstruction algorithms should be localizable and obey certain local average momentum balance properties.
An alternative approach consists in the use of variational formulations involving the stress as an independent variable which is approximated directly in suitable $H(div)$-conforming finite element spaces. The standard mixed finite element (see e.g. [3])

approach leads then to a saddle-point problem, in which the momentum balance is approximated in an optimal way, if appropriate finite element combinations are used. However, the construction of those finite element spaces is challenging, since a stability condition between the mixed spaces has to be established.
In order to avoid the complexity of this stability condition, a positive definite system can be obtained by minimizing the residuals in the partial differential equations. Using the L^2-norm leads to the Least-Squares method (see e.g. [1]), which provides the advantage of an inherent a posteriori error estimator. Due to the strong connection of this stress approximation to that obtained from a mixed formulation, the error associated with the momentum balance can be proved to be of higher order than the overall error of the least-squares approach. This implies that the favorable conservation properties of the dual-based mixed methods and the error control of the least squares method can be combined.
On domains with curved boundaries, stress approximations in Raviart-Thomas needs to be produced in the parametric Raviart-Thomas spaces studied in [2]. The use of this framework and of the actual configuration allows to extend the linear models to the nonlinear case for hyperelastic material, involving geometrical and material nonlinearities. This leads to a nonlinear mixed formulation with linear constraint, in which the symmetry of the stress tensor can be preserved.

1. F. Bertrand, S. Münzenmaier, and G. Starke, *First-Order System Least Squares on Curved Boundaries: Higher-order Raviart-Thomas Elements.* SIAM J. Numer. Anal. 52.6 (2014): 3165-3180.

2. P. Bochev and M. Gunzburger, *Least-Squares Finite Element Methods*, Springer, New York, 2009.

3. D. Boffi, F. Brezzi, and M. Fortin, *Mixed Finite Element Methods and Applications.* Springer-Verlag, Heidelberg, 2013.

Challenges of Stability Analysis using mixed FEM

N. Viebahn (University Duisburg-Essen), J. Schröder (University Duisburg-Essen), P. Wriggers (Leibniz Universität Hannover), F. Auricchio (University of Pavia) 17:30

The determination of critical loads and possible bifurcation points is a major subject in engineering applications and is often executed by means of a FE analysis. In case of classical non-linear finite element formulations, which are solely based on displacements, the singular values of the global stiffness matrix define the critical loads. These critical loads are associated to physically unstable states such as bifurcations. However, when constraints like incompressibility are present, pure displacement based finite elements have well known drawbacks, as for example locking or oscillating stress fields, see e.g. [1] and [2]. Mixed formulations circumvent these problems, see [3].
In the considered mixed forms, the potential includes a constraint related to incompressibility. Unfortunately, the resulting saddle-point structure of the discrete system leads to

indefinite systems of equations, which prohibits the application of the classical schemes for the determination of critical loads. Thus, the reliable prediction of critical load cases is still a challenging task, in the framework of mixed FEM. Furthermore, Auricchio et al. [4] showed that the choice of the incompressibility constraint could lead to unstable numerical behavior in case of classical two-field formulations.
In the proposed work two- and three-field formulations are investigated with respect to their ability of the correct determination of critical loads. Furthermore a consistent two-field formulation is presented, which is able to determine the correct critical loads, independent from the choice of the incompressibility constraint.
The proposed work is developed jointly together with K. Steeger.
The authors acknowledge support by the Deutsche Forschungsgemeinschaft in the Priority Program 1748 “Novel finite elements for anisotropic media at finite strain” (SCHR 570/23-1) (WR 19/50-1).

[1] I. Babuska, M. Suri, *Locking Effects in the Finite Element Approximation*, Numer. Math. 62 (1992), 439–463.
[2] K.J. Bathe, *Finite Element Procedures*, Prentice Hall, Englewood Cliffs (1996).
[3] D. Boffi, F. Brezzi, M. Fortin, *Mixed Finite Element Methods and Applications*, Springer Series in Computational Mathematics, vol. 44 (2013).
[4] F. Auricchio, L. Beirao da Veiga, C. Lovadina, A. Reali, R.L. Taylor, P. Wriggers *Approximation of incompressible large deformation elastic problems: some unresolved issues*, Computational Mechanics 52 (2010) 1153–1167.

A new regularization technique for geometrically nonlinear crystal plasticity implemented into a new discontinuous Galerkin element formulation

A. Alipour (Institute of Applied Mechanics, RWTH Aachen University), S. Wulfinghoff (Institute of Applied Mechanics, RWTH Aachen University), B. Svendsen (Material Mechanics, RWTH Aachen University), S. Reese (Institute of Applied Mechanics, RWTH Aachen University) 17:50

A new regularization technique for single crystal viscoplasticity is presented and implemented into a discontinuous Galerkin (DG) framework. Although single crystal plasticity has been extensively studied, its examination with the new regularization method in combination with a DG formulation allows to achieve a very simple implementation into existing finite element codes leading to a numericallly efficient, robust and locking-free model. To this end, DG quadrilateral elements with homogeneous deformation gradient are applied. As an example, the finite plastic deformation of a 2D oligocrystal is investigated under uniaxial load.

Comparative study of higher order mixed finite elements with different approximations of the minors of deformation tensors

A. Kraus (Leibniz Universität Hannover), P. Wriggers (Leibniz Universität Hannover) 18:10

In spite of the evolution of the finite element method in the last decades the development of new computational methods is required for the reliable simulation of modern high-tech materials. Fibre reinforced materials in particular exhibit strong anisotropy due to high differences in stiffness of the fibres and the matrix material leading to locking phenomena. In order to overcome these difficulties a novel computational formulation has been proposed by Schröder et al. [1] and has been extended by Bonet et al. [2].
In the current work the formulation of Schröder et al. [1] and Bonet et al. [2] is implemented. The computational performance of the proposed formulation is compared to established finite element formulations, considering different discretization schemes.

S 18 : Numerical methods of differential equations

Friday 09:00 - 11:00 Coudraystr. 11C, Room 202

Splitting Methods for Constrained Diffusion-Reaction Systems

R. Altmann (TU Berlin), A. Ostermann (University of Innsbruck) 09:00

We consider nonlinear diffusion-reaction systems which have an additional constraint such as having a prescribed integral mean. With the help of Lie and Strang splitting we would like to treat the nonlinearity separately. This means that the time integration is reduced to the solution of a linear constrained system and a nonlinear ODE.
However, Strang splitting suffers from order reduction which limits its efficiency. This is caused by the fact that the nonlinear subsystem produces inconsistent initial values for the constrained subsystem. In this talk we show that the incorporation of an additional correction term resolves this problem without increasing the computational costs.

Split Form Discontinuous Galerkin Framework Applied to Under-Resolved Turbulence

A. Winters (Universität zu Köln) 09:20

When approximating non-linear PDEs, such as the compressible Navier-Stokes equations, on discrete nodal grids, aliasing due to interpolation of non-linear fluxes can cause large errors that may drive instabilities. An interesting approach to decrease the negative effect of such aliasing errors, used primarily in the finite difference community, is to reformulate the non-linearities in different, but equivalent forms. Instead of using the conservative form of the PDE it is possible to use the advective form by applying the chain rule. It is also possible to use an arbitrary mix between those two formulations and introduce split formulations. By careful choice of such a reformulation it is possible to enhance the stability of finite difference discretizations. Many questions arise, especially if the resulting method is still fully conservative, although it is based on non-conservative forms of the underlying PDEs.
In this talk, we show how to incorporate the idea of different split forms of the compress-

ible Euler equations into the discontinuous Galerkin ansatz with the summation-by-parts (SBP) property. We show how to recover famous splitting formulations such as the Kennedy and Gruber splitting. We also demonstrate that these novel DG schemes are still fully conservative and that with these special formulations the non-linear stability for unresolved flows, such as turbulence, is highly enhanced. Lastly, we evaluate of the accuracy and fidelity of high-order split form dealiasing compared directly to consistent/over- integration for the inviscid Taylor-Green vortex (TGV).
Mathematics Subject Classification (2010): 65M60, 76F65

Conservative and Stable Degree Preserving SBP Finite Difference Operators for Non-Conforming Meshes

L. Friedrich (Universität zu Köln), G. Gassner, A. Winters (Universität zu Köln) 09:40

Non-conforming numerical approximations offer increased flexibility for applications that require high resolution in a localized area of the computational domain or near complex geometries. Two key properties for non-conforming methods to be applicable to real world applications are conservation and energy stability. The summation-by-parts (SBP) property, which certain finite-difference and discontinuous Galerkin methods have, finds success for the numerical approximation of hyperbolic conservation laws, because the proofs of energy stability and conservation can discretely mimic the continuous energy analysis of partial differential equations. In addition, SBP methods can be developed with high-order accuracy, which is useful for simulations that contain multiple spatial and temporal scales. However, existing non-conforming SBP schemes result in a reduction of the overall degree of the scheme, which leads to a reduction in the order of the solution error. This loss of degree is due to the particular interface coupling through a simultaneous-approximation-term (SAT).
We present a novel class of SBP-SAT operators that maintain conservation, energy stability, and have no loss of the degree of the scheme for non-conforming approximations. The new degree preserving discretizations require an ansatz that the norm matrix of the SBP operator is of a degree >2p, in contrast to, for example, classical finite difference SBP operators, where the norm matrix is 2p- 1 accurate.
Mathematics Subject Classification (2010): 65M06

Linearly Implicit Extrapolation Methods for Density Driven Flow

A. Naegel (Goethe-Universität Frankfurt am Main), P. Deuflhard (Beijing University of Technology), G. Wittum (Goethe-Universität Frankfurt am Main) 10:00

Many problems in porous media science and geophysics comprise interactions of processes, and are typically formulated as a system of coupled PDEs. In most cases, these systems are transient and non-linear. Developing efficient solvers is a delicate task, since one needs to must combine suitable schemes for (i) time integration, (ii) linearization, and (iii) (geometric and/or algebraic) multilevel solvers, finally being employed in a (iv)

parallel computing environment.
In this presentation we focus on the problem class of density-driven-flow of brine in a porous media. Previous studies, e.g. [1], investigated different non-linear solvers for this problem class. As the governing equations form a differential algebraic equation of index 1, linear implicit extrapolation methods [2, 3] are applicable. It is one striking feature of these methods, that inexact approximations of the Jacobian are admissible, when used as a so called W-method. We investigate different approximations and classify, which are the most favourable w.r.t. the computational effort. We present numerical experiments, report on results, and provide examples where these methods significantly improved efficiency, thus allowing to address new sets of problems.

[1] A. Nägel, A. Vogel, G. Wittum: 'Evaluating linear and nonlinear solvers for density driven flow', Computer Methods in Applied Mechanics and Engineering, 292 (2015), 3-15

[2] P. Deuflhard, U. Nowak: 'Extrapolation integrators for quasilinear implicit ODEs'. In: P. Deuflhard, B. Engquist (eds.), Large-Scale Scientific Computing (1987). Birkhauser, Boston.

[3] P. Deuflhard, E. Hairer, J. Zugck: 'One step and extrapolation methods for differential-algebraic systems', Num. Math. 51 (1987) 501-516.

Stability of a family of flux-correction methods as a remedy against overshoot in unsteady flow computation

H. Niessner (NiMa) 10:20

Still Lax-Wendroff schemes are occasionally used calculating one-dimensional flow. Supplementary flux-correction allows to reduce or even prevent unphysical overshoot occuring with discontinuous initial conditions. There is a a whole family of variants [1] based on damping or smoothing with different stability limits, which will be considered here in more detail.

[1] H. Niessner, T. Bulaty in H. Viviand(ed) "Proc. 4^{th} GAMM-Conf. Num. Meth. in Fluid Mech." Vieweg 1982, pp241-250.

S 18 : Numerical methods of differential equations

Friday 11:30 - 13:30 Coudraystr. 11C, Room 202

Efficient Ritz-Galerkin Discretization of PDE's with Variable Coefficients in arbitrary Dimensions using Sparse Grids

C. Pflaum (Friedrich-Alexander-Universität Erlangen-Nürnberg) 11:30

Sparse grids can be used to discretize elliptic differential equations of second order on a d-dimensional cube. Using the Ritz-Galerkin discretization, one obtains a linear equation system with $O(N(\log N)^{d-1})$ unknowns. The corresponding discretization error is $O(N^{-1}(\log N)^{d-1})$ in the H^1-norm. A major difficulty in using this sparse grid discretization is the complexity of the related stiffness matrix. To reduce the complexity of the sparse grid discretization matrix, we apply prewavelets and a discretization with semi-orthogonality. Stability and optimal convergence of this discretization is proved with respect to the H^1-norm for the Helmholtz equation with variable coefficients for arbitrary dimension d (see [1]). Furthermore, a recursive algorithm is presented, which performs a matrix vector multiplication with the stiffness matrix by $O(N(\log N)^{d-1})$ operations. Simulation results up to level 10 are presented for a 6-dimensional Helmholtz problem with variable coefficients. The simulation results show an optimal sparse grid convergence behavior. The condition number of the linear equation system is less than 10. This means only a few cg-iterations are need to obtain a small algebraic error. At least simulation results are presented for Poisson's equation on a 3-dimensional curvilinear bounded domain. Simulation results show optimal convergence behavior with respect to L^2-norm.

[1] C. Pflaum and R. Hartmann, A Sparse Grid Discretization of the Helmholtz Equation with Variable Coefficients in High Dimensions, SINUM, 2016.

Adaptive multiscale methods for elliptic PDEs

M. Bauer (Universität Bayreuth) 11:50

We consider an adaptive method based on positive definit functions, especially radial basis functions. Our goal is the numerical solution of elliptic partial differential equations on bounded domains for a specified accuracy. The construction of the approximate solution uses the information of several increasingly ordered fine meshes, on which the kernel function is successively smaller scaled. Furthermore we employ symmetric collocation on each level, in order to get the solution of the underlying discretized PDE on each level. Because of the set up of the multiscale method, the compactly supported radial basis functions are preferred as kernel functions.

The task of the adaptive elements, which are built in, is the generation of the finer meshes from step to step. This refinement is controlled for example by the residual of the approximated solution. In addition to the general ideas of the adaptive multiscale method, we have a look at the convergence theory. In this context, it can be shown, that the convergence is linear in the number of levels.

A few numerical examples at the end of the talk demonstrate the convergence result and the performance of this adaptive method.

A High Order Galerkin Method for the Approximation of Contour Integrals

K. Schmidt (BTU Cottbus-Senftenberg & Technische Universität Berlin), H. Heumann (INRIA Sophia Antipolis & Université de Nice Sophia Antipolis), L. Drescher (ETH Zürich) 12:10

We introduce a novel method to compute approximations of contour integrals

$$g_{f,\psi}(y) := \int\limits_{\{\mathbf{x}\in\Omega,\,\psi(\mathbf{x})=y\}} f(\mathbf{x})\,\mathrm{d}s(\mathbf{x}) \tag{6.13}$$

in some bounded domain $\Omega \in \mathbb{R}^d$, $d = 2, 3$ and some level set function ψ with $0 \leq \psi(\mathbf{x}) \leq 1$.
The new method is based on the coarea formula in combination with a Galerkin projection leading to an approximation of the function $g_{f,\psi} \in L^2(0,1)$

$$\int_0^1 g_{f,\psi}(y)\lambda(y)\mathrm{d}y = \int_\Omega f(\mathbf{x})|\nabla\psi(\mathbf{x})|\lambda(\psi(\mathbf{x}))\,\mathrm{d}\mathbf{x} \quad \forall\,\lambda \in L^2(0,1)\,. \tag{6.14}$$

As such it fits seamlessly into the spirit of hp/spectral finite element methods and circumvents the expensive and technical computation of contours. Only integrals over the domain Ω have to be evaluated.
We provide convergence estimates showing that a high order convergence can be achieved provided that the data is sufficiently smooth. Moreover, we analyze the contribution to the discretization error if an approximated level set function ψ_h, *e.g.* a Galerkin approximation of ψ, is used.
The theoretical results are supplemented by numerical experiments and an example application for plasma modeling in nuclear fusion.

[1] H. Federer, *Geometric measure theory*, Die Grundlehren der mathematischen Wissenschaften, Band 153, Springer-Verlag New York Inc., New York, 1969.

[2] H. Heumann, L. Drescher and K. Schmidt, *A High Order Method for Contour Integrals with an Application to Plasma Modeling in Nuclear Fusion*, Research Report RR-8948, INRIA Sophia Antipolis - Méditerranée, CASTOR. 2016. `https://hal.inria.fr/hal-01354031`.

Solution Representation and Approximation of Differential Sylvester Equation

M. Behr (Max Planck Institute for Dynamics of Complex Technical Systems), P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems), J. Heiland (Max Planck Institute for Dynamics of Complex Technical Systems) 12:30

We consider the autonomous differential Sylvester equation. The differential Lyapunov equation as a special case of the differential Sylvester equation as well as the algebraic ones appear in different fields of applied mathematics like control theory, system theory and model order reduction. The numerical solution of these equations needs a large amount of storage. This motivates us to summarize known solution formulas for these equations and discuss approximations.

In this talk, we illustrate how to apply the spectral theorem for normal operators to the Sylvester operator $\mathcal{S}(X) = AX+XB$ and derive a formula for a suitable induced operator norm $\|\mathcal{S}\|$ based on the spectrum of A and B. The spectral decomposition enables functional calculus for $\mathcal{S}$. In view of numerical algorithms, We identify Krylov subspaces using Taylor series and derive projection techniques to approximate the solution.

On discrete pseudo-differential operators and approximate solution of related equations

A. Vasilyev (Belgorod National Research University), V. Vasilyev (Belgorod National Research University) 12:50

We introduce a discrete pseudo-differential operator in appropriate discrete functional spaces and study invertibility properties for such simplest operators in certain canonical domains of an Euclidean space. We construct special projectors for studying these operators in dependence on a type of canonical domain and show how these operators are related to special boundary value problems for holomorphic functions of one and several variables. Also we obtain some comparison results between discrete and continual cases. Some preliminary studies for simplest operators, equations and boundary value problems were obtained in [1, 2, 3, 4, 5].

[1] Vasilyev, A.V., Vasilyev, V.B. "On solvability of some difference-discrete equations", *Opusc. Math.*, Vol. 36, No. 4, pp. 525–539, 2016.

[2] Vasilyev, A.V., Vasilyev, V.B. "Difference equations in a multidimensional space", *Math. Model. Anal.*, V. 21, No. 3, pp. 336–349, 2016.

[3] Vasilyev A.V., Vasilyev V.B. "Difference equations and boundary value problems", In: Differential and Difference Equations and Applications. *Springer Proc. Math. & Stat.* V. 164, pp. 421–432, 2016.

[4] Vasilyev A.V., Vasilyev V.B. "On finite discrete operators and equations", *Proc. Appl. Math. Mech.*, V. 16, Issue 1, pp. 771–772, 2016.

[5] Vasilyev V.B. "Discrete equations and periodic wave factorization", *AIP Conference Proceedings*, V.1759, 0200126, 2016.

Waveform-relaxation methods for distributed neural network simulations including gap junctions

J. Hahne 13:10

Contemporary simulation technology for neuronal networks enables the simulation of brain-scale networks using dimensionless spiking point-neuron models described by ODEs. The high level of abstraction in these models permits the distributed and independent solution of single-neuron dynamics for relatively long intervals, minimizing communication between compute nodes. This is however only true for simulations with only chemical

synapses: Electrical coupling between cells via so called gap junctions requires an instantaneous interaction between the coupled neurons, effectively coupling the dynamics (thus ODE-systems) of the connected neurons. In this talk we present an approach based on a waveform relaxation technique that enables current spiking simulators to simulate networks including gap junctions with high accuracy, while keeping the delayed communication strategy, that is crucial for scalability and performance.

S 19: Optimization of differential equations

Organizers: Ira Neitzel (Uni Bonn)
Johannes Pfefferer (Technische Universität München)

S 19 : Optimization of differential equations

Thursday 14:00 - 16:00 Coudraystr. 13B, 2nd floor, Room 208
Chair: Johannes Pfefferer (TU München)

Parallel-in-Time Methods for Parabolic Optimal Control Problems

S. Götschel (Zuse Institute Berlin), M. Minion (Lawrence Berkeley National Laboratory) 14:00

For the solution of optimal control problems governed by parabolic PDEs, methods working on the reduced objective functional are often employed to avoid a full spatio-temporal discretization of the problem. The evaluation of the reduced gradient requires one solve of the state equation forward in time, and one backward solve of the adjoint equation.
Time-parallel methods for the solution of time-dependent partial differential equations are receiving increasing interest in recent years to make use of additional concurrency when the scaling limit of space-parallelization is reached. There, iterative multilevel schemes such as PFASST ("Parallel Full Approximation Scheme in Space and Time") [1, 2] are currently state of the art and achieve a significant parallel efficiency of more than 50%.
In this talk, we investigate two approaches to use PFASST for the solution of parabolic optimal control problems. We discuss benefits and difficulties, and present numerical examples.

Keywords: optimal control, parabolic PDEs, parallel-in-time, PFASST
MSC 2000: 35K58, 49M05, 65M70, 65Y05

[1] M. L. Minion, R. Speck, M. Bolten, M. Emmett, D. Ruprecht, Interweaving PFASST and parallel multigrid, SIAM J. Sci. Comput. 37(5), S244–S263, 2015.

[2] M. Emmet, M. Minion. Toward an efficient parallel in time method for partial differential equations. Comm. Appl. Math. Comp. Sci. 7(1), 105–132, 2012.

Optimal control of a rate-independent evolution equation via viscous regularization

D. Wachsmuth (Universität Würzburg), G. Wachsmuth (TU Chemnitz), U. Stefanelli 14:20

We study the optimal control of a rate-independent system that is driven by a convex quadratic energy. Since the associated solution mapping is non-smooth, the analysis of such control problems is challenging. In order to derive optimality conditions, we study the regularization of the problem via a smoothing of the dissipation potential and via the addition of some viscosity. The resulting regularized optimal control problem is analyzed. By driving the regularization parameter to zero, we obtain a necessary optimality condition for the original, non-smooth problem.

A priori error estimates for space-time finite element discretization of parabolic time-optimal control problems

L. Bonifacius (TU München), K. Pieper, B. Vexler 14:40

We consider the following time-optimal control problem subject to a linear parabolic equation,

$$\text{Minimize } j(T,q) := T + \frac{\alpha}{2}\int_0^T \|q(t)\|^2_{L^2(\Omega)}\mathrm{d}t,$$

$$\begin{aligned} T > 0,\ q \in Q_{ad}, & \\ \partial_t u + Au = Bq, & \quad \text{in } (0,T)\times\Omega, \\ u(0) = u_0, & \quad \text{in } \Omega, \\ \|u(T) - u_d\|_{L^2(\Omega)} \le \delta, & \end{aligned} \tag{P}$$

with desired terminal state $u_d \in L^2(\Omega)$ and given $\delta > 0$. Moreover, Q_{ad} denotes the set of admissible controls and $\alpha > 0$ the regularization parameter.
Our aim is the numerical analysis for finite element discretizations of (P). It is worth mentioning that (P) is non-convex, possesses a non-linear dependence on T and is subject to state constraints. For these reasons the existence of Lagrange multipliers is non-trivial. Thus, we first study the stability of the optimization problem with respect to perturbations of δ. Based on the concept of weak invariance, we derive a condition that guarantees the existence of qualified optimality conditions. We emphasize that this condition can be verified without knowing the optimal solution. Several examples will be given.
Turning to the numerical solution, we consider a discontinuous Galerkin discretization scheme in time and a continuous Galerkin scheme in space. The main novelty are *a priori* discretization error estimates of optimal order under the hypothesis of second order sufficient optimality conditions.

Error estimates for Dirichlet control problems on boundary concentrated meshes

M. Winkler (Universität der Bundeswehr München), J. Pfefferer (Technische Universität München) 15:00

In this talk we present new error estimates for the numerical approximation of an optimal control problem involving the Laplace equation as side constraint, and the boundary trace of the state is the control variable. So far, the standard approach was to use a piecewise linear finite element approximation of control, state and adjoint state on a sequence of quasi-uniform meshes, or meshes that are refined locally towards singular points e. g. corners of polygonal domains. This approach leads to at most linear convergence of the approximate control in the $L^2(\Gamma)$-norm. In our approach we use meshes that are locally refined towards the boundary. Although the computational cost does not increase significantly, the accuracy of the discrete controls is improved and one obtains even quadratic convergence on smooth domains. This result remains true for polygonal domains when the interior angles at the corner points are less than $120°$. For larger angles the corner singularities reduce the regularity and hence also the convergence rate. This predicted behavior is confirmed in our numerical experiments.
When tracing through the proofs of these estimates it becomes clear that the challenging step is to show an error estimate for the Ritz-projection of the adjoint state measured in a special $L^2(\Omega)$-norm which contains the distance towards the boundary as weight function. As the vertices in the domain cause also singularities, we have to deal with regularity results in weighted Sobolev spaces containing additionally the distance to the vertices as weight functions. To show sharp error estimates we extend a technique that is used to prove local maximum norm estimates, more precisely, we apply a combination of dyadic decompositions with respect to the boundary and the vertices of the computational domain to capture the influence of both types of singularities exactly.

A semilinear parabolic problem with a directional sparsity functional

A. Rösch (Universität Duisburg-Essen), E. Casas (Universidad de Cantabria), M. Mateos (Universidad de Oviedo) 15:20

We discuss a semilinear optimal control problem with a functional forcing directional sparsity. Existence of optimal solutions can be shown in a non-standard way. Second-order sufficient optimality conditions are derived. We present a priori error estimates for a finite element discretization and some numerical experiments.

S 19 : Optimization of differential equations

Thursday 16:30 - 18:30 Coudraystr. 13B, 2nd floor, Room 208
Chair: Anton Schiela (Universität Bayreuth)

Parameter estimation with reduced basis methods for elliptic differential equations

A. Lukassen (TU Darmstadt), M. Kiehl (TU Darmstadt) 16:30

In this paper a new method for parameter estimation for elliptic partial differential equations is introduced. Parameter estimation includes minimizing an objective function, which is a measure for the difference between the parameter-dependent solution of the differential equation and some given data. We assume, that the given data results in a good approximation of the state of the system. In order to evaluate the objective function the solution of a differential equation has to be computed and hence, a large system of linear equations has to be solved. Minimization methods involve many evaluations of the objective function and therefore, the differential equation has to be solved multiple times. Thus, the computing time for parameter estimation can be large. Reduced basis methods were developed in order to reduce the computational effort of solving these differential equations multiple times. We use the given approximation of the state of the system as reduced basis and omit computing any snapshots. Therefore, our approach decreases the effort of the offline phase drastically. Furthermore, the dimension of the reduced system is one and thus, the dimension of the reduced system is much smaller than the dimension of other approaches. However, the obtained reduced model is just a good approximation close to the given data. Hence, the reduced system can lead to large errors for parameter sets, which correspond to solutions far away from the given approximation of the state of the system. In order to prevent convergence of the parameter estimator to such a parameter set we use a penalty function, which penalises the approximation error between the full and the reduced system.

Independent parameter identification in elliptic partial differential equations

Q. Tran (University of Hamburg) 16:50

In this talk I would like to present the inverse problem of identifying simultaneously the diffusion matrix, source term and boundary condition in the Neumann boundary value problem for an elliptic partial differential equation from a measurement data, which is weaker than required of the exact state. A variational method based on energy functions with Tikhonov regularization is here proposed to treat the identification problem. We discretize the PDE with the finite elements and prove the convergence as well as analyse error bounds of this approach.

[1] Hào D N and Quyen T N T(2010), Convergence rates for Tikhonov regularization of coefficient identification problems in Laplace-type equations, Inverse Problems 26, 125014 (23pp).

[2] Hào D N and Quyen T N T(2012), Convergence rates for Tikhonov regularization of a two-coefficient identification problem in an elliptic boundary value problem, Numerische Mathematik 120, 45–77.
[3] Hinze M and Quyen T N T(2016), Matrix coefficient identification in an elliptic equation with the convex energy functional method, Inverse problems 32, 085007 (29pp).

Parameter Estimation for Periodic Solutions of Climate Models

T. Slawig (Kiel University) 17:10

Parameter estimation problems for climate models are often conducted for periodic solutions, i.e. steady annual cycles in the climate system. We present different strategies for these kind of problems, including methods from optimal control and uncertainty quantification. Special focus is on the high computational effort of the underlying models and thus on options to obtain reduced or surrogate models as well as to reduce cputime by techniques from computer science. We further discuss different forms of cost functionals in the parameter optimization process that take account for lack of existence and uniqueness results for the underlying state equations. The main examples are models for simulation of the global carbon cycle.

Mathematical Degradation Modeling for Metal Films

B. Pedretscher (KAI Kompetenzzentrum Automobil- u. Industrieelektronik GmbH), B. Kaltenbacher (Alpen-Adria-Universität Klagenfurt), O. Bluder (KAI Kompetenzzentrum Automobil- u. Industrieelektronik GmbH) 17:30

In automotive industry, reliability analysis of smart power semiconductor devices is obligatory. To deduce the devices' robustness lifetime tests are used. Due to limited resources, thorough investigations can only be performed for a representative sample of devices. Based on this data set the lifetime is predicted, which is indispensable for today's semiconductor industry.
Proper lifetime modeling requires extensive analysis of the degradation mechanism. In this work, the metal degradation of a bi-layer test structure (metal on substrate) is studied. Degradation means the nucleation, growth and coalescence of voids, causing crack formation and propagation. To model this process a state space approach is proposed. The state equations are formulated as stochastic differential equations (SDEs), since the atomistic mechanisms causing elastic-plastic deformation are interpreted as diffusional activities with drift. More specific, the relation between diffusion including transport and the forward Kolmogorov equation motivates the usage of stochastic processes to describe the evolution of the microstructural heterogeneity in the metallization.
Besides developing a physical meaningful degradation model, the choice of an efficient numerical method to estimate the parameters of the inverse problem is complex due to ill-posedness and rare measurements. To address these challenges, we follow an approach by Dunker and Hohage of 2014, where parameter identification in SDEs is performed on basis of the corresponding Kolmogorov equation. The mentioned approach needs to be adapted to our application. Firstly, a stochastically consistent cost functional is

defined, taking into account the different type of measurements and secondly, instead of estimating a function, we have to recover a finite set of model parameters. For computational optimization an adjoint technique is proposed to compute the gradient of the likelihood.

Speed Profile Generation based on geo-referenced Data using Optimal Control Methods

M. Burger (Fraunhofer Institut für Techno- und Wirtschaftsmathematik), 17:50
M. Speckert (Fraunhofer Institut für Techno- und Wirtschaftsmathematik)

Speed profiles are an important and characteristic factor concerning dynamic loads of a vehicle as well as energy and resource efficiency. Thus, it is natural to aim for speed profile generation by simulation, based on specified route data and driver and vehicle characteristics, in order to analyze and to evaluate the mentioned criteria early in the development process.

We present and discuss an approach to compute speed profiles on given routes. The computation procedure is based on a longitudinal dynamics model of the considered vehicle, which includes all relevant parameters to estimate speed profiles, such as mass, engine power, air and rolling resistance coefficients, transmission ratios etc. Mathematically, the model is given as ordinary differential equation, its inputs are driving torques or forces and, if considered, a gear selection. The driver is modelled essentially by its expected acceleration behavior. Traffic is included by an expected spatial density (vehicles per kilometer) and leads through a safety-distance rule to speed limits. Both driver behavior and traffic are modelled by a stochastic process to obtain realistic profiles. In addition to the mentioned factors, geo-referenced data of the considered route essentially influences the speed profile. For the considered route, we obtain from a digital map, which is augmented by altitude information, slope and curvature data as well as information about crossroads, traffic-lights, traffic-signs and legal speed limits. All this information leads to route depend speed- and acceleration constraints.

Finally, to compute a speed profile, certain optimality criteria are formulated - for instance, driving in minimal time, with minimal consumption, following a desired profile or driving with a certain behavior such as maximal comfort. Naturally, weighted combinations of all these criteria can be modelled. We end up with a constrained optimal control problem governed by an ODE; if the gear selection is considered as input as well, the problem is of mixed-integer type. After discretization, the problem is solved numerically by a dynamic programming algorithm using Bellman's principle of optimality. We discuss variants of that approach concerning aspects of accuracy, efficiency and stability.

The resulting speed profiles can be used to analyze the impact of different driver types, different vehicle properties and last not least to compare different regions in the world, e.g., with respect to expected loads and expected consumption for certain vehicle classes

and driver types.

Classification according to MSC2010: 49J15, 49N90, 90C11, 90C90.

S 19 : Optimization of differential equations

Friday 09:00 - 11:00 Coudraystr. 13B, 2nd floor, Room 208
Chair: Arnd Rösch (Universität Duisburg-Essen)

Shape sensitivity analysis for CFD optimization using continuous adjoint method with applications to wind turbines

R. Najian Asl (Technische Universität München), S. Shayegan (Technische Universität München), K. Bletzinger (Technische Universität München) 09:00

Optimization of large-scale rotary mechanical devices like wind turbine requires time-dependent analysis. The computational cost of time-dependent approaches is considerably high for practical problems in engineering. However, any flow problem could be formulated in any reference frame and solved in that frame afterwards, as long as the boundary conditions are kept consistent. By switching to a moving reference frame, a flow field which is unsteady in the stationary (inertial) frame could be cast as a steady field with respect to the moving frame. Here we present a continuous adjoint-based shape sensitivity analysis for incompressible and rotating flows which are formulated in a reference frame rotating with a constant angular velocity. This permits to perform a steady-state optimization which costs only two fluid and adjoint converged solutions at each optimization iteration, which is not the case in unsteady gradient-based optimization. Having in mind relevant applications, different objective functions are used and respective adjoint boundary conditions are developed specifically for shape design optimization, like power production maximization and total drag minimization. Primal and adjoint solvers are implemented in OpenFOAM environment and coupled to the in-house optimizer code Carat for node-based shape optimization.

Adjoint based topology optimization of conjugate heat transfer systems

S. Goeke (University of Kassel), O. Wünsch (University of Kassel) 09:20

For many industrial applications the shape and topology of cooling channels is of significant importance for the overall cooling performance. This performance is usually a compromise between an increase in heat flux or temperature uniformity and maintaining a low pressure loss within the system. Gradient based optimization methods promise high optimization speed if the sensitivites with respect to the objective functions can be computed effortlessly. The adjoint method offers a computational cost that is independent of the degrees of freedom. The sensitivity map calculated with this approach is used as a local criterion to decide whether the fluid or solid cell is favourable for

the current objective. Gradient based topology optimization of fluid dynamic systems using the continuous adjoint approach was first presented in [1]. In this contribution the continuous adjoint equations are extended to include conjugate heat transfer. The adjoint energy equations and boundary conditions for the fluid and solid domain are derived and implemented into a novel solver within the OpenFOAM environment. The applicability of this method is tested for two dimensional cooling channels with fixed inlet and outlet positions. A uniformity objective function for the surface temperature of the solid domain is chosen and the adjoint flow variables analysed. The accuracy of the obtained sensitivities is compared to ones obtained using a finite difference method.

[1] Othmer, C.: A continuous adjoint formulation for the computation of topological and surface sensitivities of ducted flows
International Journal for Numerical Methods in Fluids 58.8, (2008) - 861-877.

Some thoughts on second order shape derivatives

A. Schiela (Universität Bayreuth) 09:40

In shape sensitivity analysis first and second order shape derivatives are defined with respect to small perturbations of the domain of interest. A puzzling property of the customary definition of the shape hessian is its lack of symmetry, which can be explained by the nonlinear nature of the applied pertubations. In this talk we propose and discuss an alternative definition of second order shape derivatives that does not suffer from the above lack of symmetry and gives true second order information to be used, e.g., in optimization algorithms.

Multiple state optimal design problems with explicit solution

M. Vrdoljak (University of Zagreb), K. Burazin (University of Osijek) 10:00

We consider multiple state optimal design problems for stationary diffusion in the case of two isotropic phases, aiming to minimize or maximize a convex combination of energies. It is well known that for problems with one state equation, for general functional, there are relaxed solutions corresponding to simple laminates at each point of the domain. As a consequence, one can write down a simpler relaxation, written only in terms of the local proportion of given materials.
In the case of multiple state equations, we shall study the relationship between an analogus simpler relaxation and the proper relaxation via homogenization theory. The simpler relaxation problem is represented by a convex-concave minimax problem and its solution can be characterised by necessary and sufficient optimality conditions. The optimality conditions are further analyzed on some examples, where the presented method enables explicit calculation of an optimal design.

Optimality Conditions for Switching Operator Differential Equations

F. Rüffler, F. Hante 10:20

We consider optimal switching of hybrid abstract evolution equations. The framework includes switching semilinear partial differential equations of parabolic or hyperbolic type, discontinuous state resets, switching costs and allows switching of the principle parts of the equations. We present first order necessary conditions for optimality with respect to switching times and discuss strategies for also optimizing the discrete mode sequence. The results are based on a hybrid adjoint calculus. Points satisfying the optimality conditions can be found using gradient decent algorithms. As an application we consider optimal open/close and on/off switching control of valves and compressors in a gas network modeled by a graph with simplified euler equations on edges and suitable coupling conditions at nodes.

S 19 : Optimization of differential equations

Friday 11:30 - 13:30 Coudraystr. 13B, 2nd floor, Room 208

Towards Riccati-Feedback Control of Complex Flows with Moving Interfaces

B. Baran (Max Planck Institute for Dynamics of Complex Technical Systems), P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems), J. Heiland (Max Planck Institute for Dynamics of Complex Technical Systems), J. Saak (Max Planck Institute for Dynamics of Complex Technical Systems) 11:30

Problems featuring moving interfaces appear in many applications. They can model solidification and melting of pure materials, crystal growth and other multi-phase problems. The control of the moving interface allows to, for example, influence production processes and, thus, the product material quality.

We consider the two-phase Stefan problem that models a solid and a liquid phase separated by the moving interface. In the liquid phase, the heat distribution is characterized by a convection-diffusion equation. The fluid flow in the liquid phase is described by the Navier–Stokes equations which introduces a differential algebraic structure to the system. The interface movement is coupled with the temperature through the Stefan condition, which adds additional algebraic constraints. Our formulation uses a sharp interface representation and we define a quadratic tracking-type cost functional as a target of a control input.

We compute an open loop optimal control for the Stefan problem using an adjoint system. For a feedback representation, we linearize the system about the trajectory defined by the open loop control. This results in a linear-quadratic regulator problem, for which we formulate the differential Riccati equation with time varying coefficients. This Riccati equation defines the corresponding feedback gain.

In this talk, we show how the differential Riccati equation is derived. Further, we

present the feedback formulation that takes into account the structure and the differential algebraic components of the problem. Also, we discuss how the complexities that come, for example, with mesh movements, can be handled in a feedback setting.

Optimal control of time-discrete two-phase flow driven by a diffuse-interface model

C. Kahle (TU München), H. Garcke, M. Hinze (Universität Hamburg) 11:50

We present results on optimal control of two-phase flows. The fluid is modeled by a thermodynamically consistent diffuse interface model proposed in [H. Abels, H. Garcke, G. Grün, Thermodynamically consistent, frame indifferent diffuse interface models for incompressible two-phase flows with different densities, M3AN, 22(3), 2012] and allows the simulation of fluids with different densities and viscosities.
In earlier work [H. Garcke, M. Hinze, C. Kahle, A stable and linear time discretization for a thermodynamically consistent model for two-phase incompressible flow, APNUM, 99, 2016] we proposed an energy stable time discretization scheme for this model that we now employ as constraint in an optimal control problem. We show existence of at solutions and derive first order neccessary optimality conditions for the time discrete optimal control problem.
The control aim is to obtain a desired distribution of the two phases in the system after some given time. For this we investigate three control actions. We use both tangential Dirichlet boundary control and distributed control where the control acts as amplitudes of given fixed controls. We further consider the inverse problem of finding an initial distribution such that the distribution after given time horizon starting from this value is close to a desired distribution.

Optimal Control of Mechanical Damage Processes

M. Holtmannspötter (Universität Duisburg-Essen), C. Meyer, A. Rösch (Universität Duisburg-Essen) 12:10

In mechanics damage models describe the behaviour of an object loaded by an external force. In addition to the deformation of the object the damage done to the material due to the deformation is of special interest.
In this talk we study an optimal control problem governed by a particular gradient enhanced damage model. After giving an overview of the models special features as well as analytic results we focus on solving the problem numerically. We will point out the difficulties arising from the model containing nonlinear and non-differentiable terms. Finally we present first numerical results.

Optimal Control of Thermoviscoplasticity

A. Stötzner (TU Chemnitz), R. Herzog (TU Chemnitz), C. Meyer 12:30

Elastoplastic deformations play a tremendous role in industrial forming. Many of these processes happen at non-isothermal conditions. Therefore, the optimization of such problems is of interest not only mathematically but also for applications.

In this talk we will present the analysis of an optimal control problem governed by a thermovisco(elasto)plastic model. We will point out the difficulties arising from the nonlinear coupling of the heat equation with the mechanical part of the model. Finally, we will discuss first numerical results.

Application of Multi-Parametric Quadratic Programming to Simulation of Deflected Wires in a Wire Saw

D. Treyer (University of Applied Sciences Northwestern Switzerland), S. Gaulocher (University of Applied Sciences Northwestern Switzerland), S. Niederberger (University of Applied Sciences Northwestern Switzerland), H. Rafael (Meyer Burger), A. Ams (TU Bergakademie Freiberg) 12:50

In the wire sawing process used in the photovoltaic industry for the production of wafers, a field of thin abrasive wires is spanned between two wire guide rollers. A silicon brick is fed into the moving wire field, deflecting the wires. The resulting contact forces cause material removal on the silicon brick, altering its kerf. A parametric model might be used to describe the material removal rate as a function of the contact forces. By considering static deflections only, the wire displacement and the contact forces between wire and silicon brick may be calculated by minimizing the potential energy of the wire. The minimization is done by solving a quadratic optimization problem, subject to a number of constraints. As a consequence, in a time domain simulation, the continuously changing contour inside the kerf requires to repeatedly solve the optimization problem.
This work aims at reducing the computational effort of repetitive optimization by applying multi-parametric quadratic programming. The present paper describes the approximation of the resulting partial derivatives by finite differences and the underlying discretization of a single wire into non-equidistant elements. Based on the formulation of the optimization problem, the application of multi-parametric quadratic programming is shown and some figures on simulation time reduction in this application scenario are given.

S 20: Dynamics and control

Organizers: Karl Worthmann (TU Ilmenau)
Matthias Müller (University of Stuttgart)

S 20 : Dynamics and control

Tuesday 14:00 - 16:00 Weimar hall, Small hall
Chair: Matthias A. Müller (Universität Stuttgart)

On the Direct Computation of the Byrnes-Isidori Normal Form

K. Röbenack (TU Dresden) 14:00

If an input-affine control system

$$\dot{x} = f(x) + g(x)u, \quad y = h(x)$$

given by the vector fields $f, g : \mathbb{R}^n \to \mathbb{R}$ and a scalar field $h : \mathbb{R}^n \to \mathbb{R}$ has a well-fined relative degree r, there exists a (local) diffeomorphism Φ transforming the system into the Byrnes-Isidori normal form. By this transformation, the system is decomposed into a r-dimensional first subsystem and a second subsystem of dimension $n-r$. An important property of the Byrnes-Isidori normal form is the fact that the differential equations of the second subsystem do not directly depend on the input u. To achieve this structure, the last $n-r$ components $\phi_{r+1}, \dots \phi_n$ of the diffeomorphism Φ must fulfill the condition

$$L_g \phi_i = 0 \quad \text{for} \quad i = r+1, \dots, n, \tag{6.15}$$

where $L_g \phi_i$ denotes the Lie derivative of the scalar field ϕ_i along the vector field g. Formally, Eq. (6.15) is a set of partial differential equations. Practically, the appropriate choice of these coordinates is left to the (experienced) user. In this note, the author suggests a direct computation based on the calculation of flows of certain vector fields.

A Canonical Form for Perspectively Unobservable LTI State-Space Systems

R. Seeber (Technische Universität Graz), N. Dourdoumas (Technische Universität Graz), M. Horn (Technische Universität Graz) 14:20

Perspective observability is an observability property for the case when only the perspective projection of a dynamical system's output is available [1]. Given an LTI system

$$\frac{\mathrm{d}\mathbf{x}}{\mathrm{d}t} = \mathbf{A}\mathbf{x}, \qquad \mathbf{y} = \mathbf{C}\mathbf{x},$$

with state vector $\mathbf{x} \in \mathbb{R}^n$ and output vector $\mathbf{y} \in \mathbb{R}^m$ this property in its simplest form—for the so-called dimension loss $d = 1$—is equivalent to an affirmative answer to the following question: Knowing only the direction of $\mathbf{y}(t)$, i.e. its projection onto the space $\mathbb{RP}^{m-1}$ consisting of all homogeneous lines in $\mathbb{R}^m$, can the direction of $\mathbf{x}(t)$ be recovered? For arbitrary dimension loss $d \geq 0$ this question is generalized to: given a linear, homogeneous differential equation

$$\frac{\mathrm{d}\mathcal{X}}{\mathrm{d}t} = \mathbf{A}\mathcal{X},$$

for a $d+1$ dimensional vector space $\mathcal{X}$, can $\mathcal{X}(t)$ be recovered from the knowledge of the vector space $\mathcal{Y}(t) = \mathbf{C}\mathcal{X}(t)$?

Based on existing criteria for deciding a system's perspective observability [2, 3, 4], this talk presents a canonical form for systems that are not perspectively observable. For $d = 0$, where the property is equivalent to the classical observability of an LTI system, this form reduces to the well-known Kalman decomposition of non-observable systems. The issue of this canonical form's (non-)uniqueness is discussed. Furthermore, structural insights gained from it and its usefulness for computing the distance of a given system to the nearest perspectively unobservable system are shown.

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Velocity Turbulences in Road-Vehicle Dynamics

W. Wedig (KIT Karlsruher Institut für Technologie) 14:40

Weakly damped vehicles which are riding on narrow-banded road profiles [1], lead with increasing band-width to resonance reductions of the vertical car vibrations [2] and additionally, to mean velocity jumps [3] when a nonlinear velocity coupling of the along and across dynamics of the vehicle is considered. Controlling the driving force of the car, the velocity of the vehicle fluctuates around a mean velocity because of the random up and down of the road profile relatively to the moving vehicle. It is clear that the fluctuations of the vehicle velocity decrease when the road surface becomes smoother.
The velocity density distribution with one peak bifurcates into bimodal densities with two peaks [4] when the driving force approaches the critical range where the vertical car vibrations are resonant. In this critical case, the velocity process of the vehicle is fluctuating around two mean values with permanent jumps between both that can't be avoided even when the excitation intensity becomes small. However, this situation is completely changed in the deterministic case when limited harmonic wave roads are applied. For small road amplitudes, the vehicle velocity remains in one mean value without any jump.
In the stochastic case, road surfaces are generated by means of dynamic models which are transformed from way to time when the vehicle rolls with constant velocity. It is shown that these dynamic road models lead to stationary Gaussian density distributions which are independent on velocity and therefore applicable for all non-negative velocities. The application of the Fokker-Planck equation allows to develop analytical approximations in the road-vehicle dynamics of interest. Finally, the applied quarter car model is extended to chains of rigidly along-coupled vehicles rolling on rough underground.
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Edge-wise funnel synchronization

S. Trenn (TU Kaiserslautern) 15:00

Recently, it was suggested in [1] to use the idea of funnel control in the context of synchronization of multi-agent systems. In that approach each agents i is able to measure the difference of its own state and the average state of its neighbours and this synchronization error $e_i(t)$ is used in the feedback law $u_i(t) = -k_i(t)e_i(t)$, where $k_i(t)$ is chosen as the typical funnel gain [2]. In [1] some preliminary results are proven and simulations indicate that this approach indeed leads to practical synchronization with prescribed transient behavior. However, the synchronized behavior does not follow the expected trajectory from the case of constant high gain feedback [3]. To recover the desired average dynamics from [3] this talk will introduce the approach of edge-wise funnel synchronization. The feedback now takes the form

$$u_i(t) = -\sum_j k_{ij}(t)(x_i(t) - x_j(t)),$$

where the index j runs over all neighbors of agent i and $k_{ij}(t)$ is the standard funnel gain for the error measured on the edge (i, j), i.e., $e_{ij}(t) = x_i(t) - x_j(t)$. With this choice the overall feedback retains an important symmetry property also present in the constant high-gain feedback approach, but lost in the approach in [1], hence the synchronization towards the predicted average dynamics is expected.

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Algebraic properties of linear time-varying systems

A. Ilchmann (TU Ilmenau), D. Dennstädt (Technische Universität Ilmenau) 15:20

We consider linear time-varying systems

$$\sum_{i=0}^{n} R_i(t)x^{(i)} = 0,$$

where the time-varying matrices $R_i(\cdot)$ are defined by means of locally convergent Puiseux series. This system class has recently been introduced by *Bourlès, Marinescu and Oberst* (2015). The behaviour, i.e. the C^∞-solution space, has a one-to-one correspondence to a factor module. The latter allows for an algebraic description of the system class. We show that the theory introduced by *Bourlès, Marinescu and Oberst* (2015) allows to characterize controllability, observability, and system equivalence in algebraic terms.

Ensemble controllability of linear parametric systems

M. Schönlein 15:40

We consider families of parameter-dependent systems

$$\frac{\partial x}{\partial t}(t,\theta) = A(\theta)x(t,\theta) + B(\theta)u(t), \quad x(0,\theta) \in \mathbb{R}^n, \theta \in \mathbf{P}$$

where P is compact interval and the matrices $A(\theta)$ and $B(\theta)$ depend continuously on the parameter $\theta \in \mathbf{P}$. The focus of this talk is on the task of steering the continuous family of initial states $\{x(0,\theta) \,|\, \theta \in \mathbf{P}\}$ in finite time arbitrarily close to a continuous family of desired terminal states $\{x^*(\theta) \,|\, \theta \in P\}$ by a single parameter independent open-loop input function u. In this case, the family $\{\big(A(\theta), B(\theta)\big) \,|\, \theta \in \mathbf{P}\}$ is called ensemble controllable. Using well-known characterizations of approximate controllability of systems in Banach spaces, this talk presents a unified approach to ensemble controllability. In addition, the talk presents necessary and sufficient conditions for ensemble controllability in terms of the matrix pair $(A(\theta), B(\theta))$.

S 20 : Dynamics and control

Tuesday 16:30 - 18:30 Weimar hall, Small hall
Chair: Stephan Trenn (TU Kaiserslautern)

Distributed measurement feedback control for dynamically coupled linear systems

N. Dmitruk (Belarusian State University) 16:30

Control problems for interacting dynamical systems has received significant attention in recent years. Various approaches have been proposed in the framework of distributed model predictive control for control of dynamically coupled and decoupled systems for stabilization, synchronization, consensus, obstacle avoidance and other control problems. Most of them rely on perfect knowledge of local system states. In this presentation we

address the case when initial and current states are not available for the control purposes, only noisy measurements are known to the local controllers. In particular, we consider a group of dynamically coupled linear systems of the form

$$\dot{x}_i = A_i x_i + \sum\nolimits_{k \in I \setminus i} A_{ik} x_k + B_i u_i, \quad x_i(0) \in X_{i0}, \ i \in I = \{1, 2, \ldots, q\}, \tag{1}$$

where x_i denotes the state of the i-th system, u_i denotes the bounded sampled-data control input; the initial state $x_i(0)$ is not exactly known. For control purposes only measurements $y_i = C_i x_i + \xi_i$ that are subject to bounded measurement errors ξ_i are available at sampling times to each system locally. Given the possibly large-scale overall system (1) subject to noisy state measurements, the control objective is to steer it robustly (i.e. for all realizations of uncertainties) in a fixed finite time to a given polytope that defines a coupling terminal constraint, while minimizing the worst-case linear terminal penalty.

In this talk, we present a distributed feedback control scheme for (1) based on distributed set-membership estimation. In particular, the distributed feedback is defined via repetitive (for every sampling instant) solution by the local controllers of some local predictive optimal control problems $\mathcal{P}_i$ in a receding horizon fashion albeit with a shrinking horizon due to the finite-time control interval. The optimal control problems $\mathcal{P}_i$ are subject to (i) guaranteed estimates of the current local state that are obtained from the local estimation problem $\mathcal{E}_i$ and (ii) some information received from all other systems of the group. As in receding horizon control, the first value of the optimal open-loop control of problem $\mathcal{P}_i$ is fed into the input of the i-th system until the next sampling instant. We discuss suitable formulations of local optimal control problems $\mathcal{P}_i$ and local estimation problems $\mathcal{E}_i$ that guarantee robust constraints satisfaction for the overall system, recursive feasibility of all local problems that are solved at each sampling time, and improvement of the terminal cost in the course of the control process. Requirements for the data communicated between the systems are also presented.

This work was supported in part by the Belarusian Republican Foundation for Fundamental Research and in part by the Institute for Systems Theory and Automatic Control, University of Stuttgart, within the joint grant 14MC-005.

Quadratic Costs do not always work in MPC

M. Müller (University of Stuttgart), K. Worthmann (TU Ilmenau) 16:50

We consider model predictive control (MPC) without terminal costs and/or constraints. Firstly, we rigorously show that MPC based on quadratic (stage/running) costs may fail, i.e., there does not exist a prediction horizon length such that a (controlled) equilibrium is asymptotically stabilized although the control system itself is, e.g., finite time controllable. Hence, stability properties of the infinite horizon optimal control problem are, in general, not preserved in MPC as long as purely quadratic costs are employed. This shows the necessity of using the stage cost as a design parameter in order to achieve asymptotic stability.

On the relation between finite and infinite horizon turnpike properties

L. Grüne (Universität Bayreuth) 17:10

The investigation of turnpike properties has a long history in optimal control. Roughly speaking, these properties formalise that optimal trajectories most of the time stay near a particular reference trajectory, which is often an equilibrium. Recently, these properties have received renewed interest, on the one hand because they simplify the synthesis of optimal controls in both ODE and PDE based control problems (for the latter see particularly recent work of Porretta/Zuazua and Trelat/Zuazua). On the other hand, they provide an important building block for understanding Model Predictive Control (MPC). Both aspects will be briefly explained in the first part of this talk.
In the literature, turnpike properties are usually formulated and analysed separately for finite or for infinite horizon optimal control problems. In this talk we show how these two variants are related. More precisely, we give conditions under which finite horizon turnpike properties imply the occurrence of infinite horizon turnpike behaviour and vice versa. We address both "qualitative" versions of the turnpike property as well as "quantitative" versions, in which the speed of convergence towards the reference is also formalised.
The talk is based on joint work with Chris Kellett and Steve Weller (University of Newcastle, Australia)

Economic model predictive control for time-varying systems

L. Grüne (University of Bayreuth), S. Pirkelmann (University of Bayreuth) 17:30

In classical model predictive control (MPC) we want to steer the system to a certain state, which is achieved by using a cost functional that penalizes the distance to either an equilibrium of the dynamical system or some optimal reference trajectory. This implies that we need to know the desired trajectory beforehand, in order to be able to actually track it.
However, in some applications the optimal reference trajectory may be unknown or cannot be computed with reasonable effort. Besides, even if we knew the optimal trajectory of the system, there would be no guarantee that the combined closed-loop solution of the MPC tracking algorithm would follow the optimal trajectory in an optimal manner.
In contrast, so called economic MPC offers the advantage of allowing for more general types of cost functionals, which enables us to directly incorporate an arbitrary performance criterion in the optimization problem itself. In particular, we do not have to provide an optimal reference, but instead the MPC algorithm will automatically determine a control input that achieves our goal.

The talk will deal with performance estimates for economic MPC in the case of time-varying system dynamics. We will use the concept of overtaking optimality to classify what we consider optimal and investigate under which assumptions we can expect optimality of the controller by means of verifying turnpike properties of the open-loop

trajectories of the MPC optimization problems.
Applications for this type of MPC arise in the energy efficient operation of buildings. As an example we consider a single room modeled by a parabolic partial differential equation. The goal is to keep the temperature of the room within a certain range, by compensating for fluctuating outside temperatures, and doing so in an energy efficient way.

Cost-to-travel functions - a new perspective on economic model predictive control

M. Müller (University of Stuttgart), B. Houska (ShanghaiTech University) 17:50

In this talk, we discuss the concept of cost-to-travel functions as a generalization of cost-to-go functions, which are often used in the context of dynamic programming as well as model predictive control. For a given (potentially nonlinear) control system, the cost-to-travel function associates with any given start and end point in the state space and any given travel duration the minimum economic cost of the associated point-to-point motion.
We discuss some properties of cost-to-travel functions and show how they can be employed (i) to provide additional insight and alternative proofs to some known results in the field of economic model predictive control (MPC) and (ii) to derive novel results in this context. In particular, we present conditions under which an m-periodic orbit of a discrete-time nonlinear system is optimal among all periodic orbits of arbitrary period length. Furthermore, we show how the closed-loop behavior of a certain economic MPC scheme with return constraints can be analyzed by studying the convergence properties of a certain block-coordinate descent method.

Multiobjective Model Predictive Control

M. Stieler (Universität Bayreuth), L. Grüne (Universität Bayreuth) 18:10

The talk deals with the question how multiobjective optimal control problems can be incorporated into the framework of model predictive control (MPC). In the literature it is common practice to optimize a weighted sum of all objectives. Thus, the well-known results for single-objective MPC apply and stability and performance of the weighted sum are easily deduced. However, performance statements on the original objectives can not be obtained this way.
In our approach we do not define such an overall objective function. Instead, we prove that choosing an 'appropriate' Pareto optimal solution to the multiobjective optimization problem in each MPC iteration yields a bounded infinite-horizon cost functional of the MPC controller for all objectives. Our findings will be illustrated based on numerical examples.

S 20 : Dynamics and control

Wednesday 14:00 - 16:00 Coudraystr. 11C, Lecture hall 1
Chair: Karl Worthmann (TU Ilmenau)

Impact of quantization on consistency of distributed model predictive control in street traffic with dynamic priority rules

T. Sprodowski (University of Bremen) 14:00

Distributed systems mainly rely on communication as a necessary condition to drive the overall system to a reference or target state. In a Multi-Agent-System with communication among the agents, this may lead to a large communication overhead. We consider, that individual targets and initializations are assigned to each agent. In such a setting, each agent predicts in every time step its own trajectory which is broadcasted among the agents as a prediction of states. Here, we evaluate the influence of quantization of communicated predicted states on the prediction coherence of each agent. The quantization is mainly motivated to reduce the necessary communication overload among the agents. We define the prediction coherence as a degree of difference of two predictions in two successive time steps. Here, we utilize the Distributed Model Predictive Control Scheme (DMPC) in a street traffic model incorporating autonomous connected vehicles. We consider an intersection whose spacial set is quantized. Different partition sizes of the spacial set are numerically examined to evaluate the prediction coherence for incorporating possible disturbances in communication. Additionally, we examine numerically the incorporation of dynamic priority order rules. The numerically examined prediction coherence gives an indication regarding robustness of the system.

Energy-optimal Swing-up of an Electro-mechanically Actuated Double Pendulum

D. Kern (TU Chemnitz), M. Groß 14:20

A control strategy for swinging up a pendubot, from its hanging to its upright position, is presented. A pendubot is a double pendulum with its base hinge actuated and its inner hinge, between the links, unactuated. This is a popular example for underactuated, nonlinear control problems. In contrast to the frequently used model of torque control, the DC-motor is included as RLC circuits of stator and armature in this paper. The armature voltage is used as input signal, while the stator voltage is fixed.
In order to compute the optimal feed-forward control Hamilton's principle is applied and discretized by a variational integrator (VI). Thus, the resulting optimal control problem is transferred into a finite-dimensional optimization problem, and solved by SQP methods. The cost function to be minimized is the consumed electrical energy needed to swing up the pendubot in a prescribed time.
In addition to the feed-forward control (offline), a feed-back controller (online) is added in order to stabilize the swing-up and the upright position. This feedback-controller is designed as linear-quadratic regulator (LQR) around the linearization of the nominal

trajectory.

Dynamics of a running gear with IRWs on curved tracks for robust control development

G. Grether (Deutsches Zentrum für Luft- und Raumfahrt (DLR)) 14:40

Within the DLR-internal project "Next Generation Train" a high-speed train with independently rotating wheels (IRWs) is developed. Due to the missing self-centering behavior of IRWs in contrast to conventional wheelsets, an active track guidance control has to be applied. The recent control structure performs well on straight tracks but the gyroscopic moments caused by the superelevation in transition curves deteriorate the controller performance significantly. To enable a robust model-based control synthesis an analytical model of a running gear with IRWs is deduced using Euler-Lagrange-equations. The established running gear model takes these track properties into account and covers in this way various track scenarios. Furthermore, the complexity of the system is reduced to allow robust control synthesis and feed forward control including model inversion. Finally, the model is discussed and validated by extensive multibody simulations applying the "DLR RailwayDynamics Library".

Optimization of ship maneuvering within the project GALILEOnautic

S. Roy (University of Bremen) 15:00

The goal of the project GALILEOnautic is to develop a system for autonomous navigation and optimal maneuvering of cooperative ships in safety-critical areas. In this context, many challenges arise in the field of optimization and control and the research presented here addresses two of them. Firstly, parameter identification is performed on four-quadrant 3DoF ship models in order to best describe the non-linear behaviour of experimental ships. The models considered are called modular. In comparison to regression models, they show the advantage of being more flexible and allow for rapid and effective changes in design. Secondly, these models are used in the computation of optimal trajectories and controls for groups of cooperative ships taking into account factors such as wind, surface water current and some geometric constraints including the limits of a harbour. For the optimization, the energy consumption of the whole fleet of ships as well as the time required to reach their goals are considered. Both these tasks of identifying model parameters and of calculating optimal ship trajectories and controls have been successfully performed using the software library WORHP, the official ESA NLP solver, and more specifically the software TransWORHP, which transcribes optimal control problems into optimization problems.

Variational integrators for open-loop and closed-loop optimal control of mechanical systems

K. Flaßkamp (Universität Bremen), C. Büskens (Universität Bremen) 15:20

In many fields of application, e.g. robotics, biomechanics, or automotive engineering,

control and optimization tasks for the underlying mechanical system arise. Those tasks can only be solved by numerical techniques. Mechanical systems exhibit special structures (energy preservation, symmetries, symplecticity) which are desirable to preserve in numerical simulation and optimization. Therefore, variational integration (VI) as a discretization method that inherently preserves system structures has gained growing interest in recent years. The focus has been on using VI for transcription in the design of direct optimal control methods and also, but rarely, for indirect control methods. In linear quadratic problems, we can derive discrete-time Riccati equations tailored to VI discretizations in order to provide closed-loop control laws. This talk focusses on local closed-loop control design based on time-varying system linearizations and the combination of open-loop and closed-loop control with variational integrators.

Motion planning with obstacle avoidance for a class of bracket generating systems

V. Grushkovskaya (University of Stuttgart), A. Zuyev (Max Planck Institute for Dynamics of Complex Technical Systems) 15:40

This work is devoted to the study of the obstacle avoidance problem for nonlinear control systems of the following form:

$$\dot{x} = \sum_{i=1}^{m} u_i f_i(x), \quad x \in D \subset \mathbb{R}^n,\ u \in \mathbb{R}^m \tag{6.16}$$

where $x = (x_1, ..., x_n)^T$, $u = (u_1, ..., u_m)^T$, $m < n$, and the vector fields $f_i \in C^2(D)$ satisfy Hörmander's condition in D, $D \subset \mathbb{R}^n$. Suppose that the closed domain D is defined as $D = \mathcal{W} \setminus \bigcup\limits_{j=1}^{N} \mathcal{O}_j$, where $\mathcal{W} \subset \mathbb{R}^n$ is a closed bounded domain, and $\mathcal{O}_j$ are domains such that $\bar{\mathcal{O}}_j \subset \mathrm{int}\mathcal{W}$, $j = \overline{1, N}$. We consider the following obstacle avoidance problem:

Given an initial point $x^0 \in \operatorname{int} D$ and a destination point $x^* \in \operatorname{int} D$, the goal is to construct an admissible control such that the corresponding solution of system (6.16) *with the initial data $x(0) = x^0$ satisfies the following conditions:*

$$x(t) \in \operatorname{int} D \ \text{ for all } \ t \geq 0, \quad x(t) \to x^* \ \text{ as } \ t \to +\infty.$$

Such problem has been the subject of many investigations, however, the most of publications in this area deals with particular classes of nonholonomic systems only. Unlike that, we develop a constructive approach for solving the obstacle avoidance problem for general step-2 bracket generating systems (6.16). The proposed control design arises from the results of papers [3, 4]. By using the Volterra series expansion of the solutions of system (6.16) with a family of trigonometric controls

$$u^{\varepsilon}(t, x) = v(x) + \sum_{(i,l) \in S} a_{il}(x) \Big\{ \cos\left(\frac{2\pi k_{il}(x)}{\varepsilon} t\right) e_i + \sin\left(\frac{2\pi k_{il}(x)}{\varepsilon} t\right) e_l \Big\} \tag{6.17}$$

we reduce the problem considered to a system of second order algebraic equations on coefficients $v(x) \in \mathbb{R}^m$, $a_{il}(x) \in \mathbb{R}$ of the control functions. The local solvability of the obtained algebraic system is proved. In system (6.17), e_i denotes the i-th unit vector in $\mathbb{R}^m$, $S \subseteq \{1, 2, ..., m\}^2$ is some set of indices, $\varepsilon > 0$ is a real parameter, and $k_{il}(x) \in \mathbb{Z} \setminus \{0\}$.
The proposed approach for solving the obstacle avoidance problem is universal in the sense that it is applicable for different classes of potential functions generating collision-free paths, e.g., artificial potential fields [1], navigation functions [2]. Moreover, different shapes of obstacles and workspace can be treated within our approach.

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S 20 : Dynamics and control

Wednesday 16:30 - 18:30 Coudraystr. 11C, Lecture hall 1
Chair: Kathrin Flaßkamp (Universität Bremen)

Comparision of a Filter- and a Model Predictive Control Based Motion Cueing Algorithm

F. Ellensohn (Technische Universität München) 16:30

Motion Cueing Algorithms (MCA) include control strategies to take account of driving simulator's restrictions concerning working space barriers and dynamic boundaries. A typical simulator consists in a motion system which exhibits three translational and rotational degrees of freedom, respectively. Its actuators are capable to realize accelerations, velocities and positions in a limited range. Based on these facts MCAs aim to generate realistic simulations of the driving movement in order to put test persons in virtual environments [Sammet, 2007].
Filter-based, classical MCAs belong to the most applied algorithms and mainly consist of linear transfer functions [Fischer, 2009]. Whereas, model predictive control algorithms rest upon a reduced model of the technical system's dynamics as well as the human perception mechanism. An optimization problem subject to the restrictions of the

motion system predicts the control variables over a time horizon [Beghi et al., 2012]. This paper depicts the strengths and weaknesses of the two stated approaches and gives an outlook why optimization based algorithms have a higher potential to improve driving simulation.

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Mathematical approaches in autonomous driving

A. Cobus (Universität Bremen), M. Rick, L. Sommer, N. Backfisch, A. Probst, M. Echim (Universität Bremen), C. Büskens (Universtität Bremen) 16:50

Autonomous driving is no longer a subject of science fiction. Instead it has become a field of highly topical developments and numerous already reached milestones. Here, research has shown that optimization and control techniques play a key role in the design of autonomous vehicles. The *Audi Autonomous Driving Cup* provides a stage for students to participate in this process. This competition, carried out in Germany, Austria and Switzerland, offers miniature vehicles of normed hardware. With these, participants are supposed to implement algorithms for autonomous handling of problems such as lane tracking, entering and exiting parking spaces, obstacle detection, adaptive cruise control, overtaking as well as turning. Here, we will take the first two applications as examples to present concepts of optimal control based on dynamical vehicle models in combination with image processing methods which we use to handle those problems.

Modal controllability and observability of different classes of vehicles

J. Edelmann (TU Wien), M. Plöchl 17:10

Modal controllability and observability has proven to be a useful measure for the effectiveness of actuators in vehicle dynamics control, e.g. [1]. With the stepwise introduction of autonomous driving functions in automobiles, redundant actuators, such as additional rear wheel steering or torque vectoring, may guarantee tracking of a desired path in case of system failure. These systems may have considerable impact on the handling characteristics of respective vehicles. Due to the inherently different system behaviour in vehicles with typical oversteer characteristics and understeer characteristics, the effectiveness of several actuators with regard to controllability may be different too.

Based on previous studies, e.g. [2], the joint modal controllability and stability measure proposed in [3] will be applied to both types of automobiles and conclusions regarding redundant actuators discussed.

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Dynamics and Nonlinear Control of a Switched Hydraulic System

S. Schröders (Karlsruher Institut für Technologie), A. Fidlin (Karlsruher Institut für Technologie), M. Köster (Karlsruher Institut für Technologie) 17:30

Because of its rapidness and high energy density, hydraulic power transmission is often used in a variety of technical applications, e.g. in clutch actuation in the automotive sector. Energy allocation in a hydraulic circuit is realized by valves, whose dynamic behaviour have not been investigated extensively from a mathematical point of view. It is known, that stability problems can occur in certain operating points, but these have not been sufficiently understood in general yet. To handle these stability problems and to improve system performance, topology of these systems is often based on long term experience, which often leads to relatively complex system structures. Another approach is to use servo valves, which allow a more advanced control of the system. Due to the non smooth behaviour of most of the valves concerning their volume flow characteristics, the development of control strategies for hydraulic systems is challenging. This might be the reason why most developed control strategies have remained linear so far, allowing only local operation in the environment of certain operating points.
In this paper, a minimal hydraulic circuit with a pressure regulation valve, a vane pump and a consumer is investigated. The model can be represented by a four state system with switched behaviour due to the non-smooth volume flow characteristic of the pressure regulation valve. The function of the circuit is to provide a certain pressure for one or several consumers, e.g. clutches or hydro motors. A stability investigation shows, that the equilibrium position of the system can become unstable for certain sets of parameters, if the valve is open. To avoid undesirable self-excited oscillations, a nonlinear control strategy, based on the input-output linearization technique, is developed and examined regarding the performance and the energy efficiency of the resulting control system.

Two Degree-Of-Freedom Online Compensation of a Piezoelectric Micro - Positioning Unit

C. Schindlbeck (Leibniz Universität Hannover), C. Pape (Leibniz Universität Hannover), E. Reithmeier (Leibniz Universität Hannover) 17:50

Due to their almost unlimited resolution and fast dynamics, piezoelectric actuators

are a common choice for mechatronic systems targeting positioning tasks with high demands on precision. However, these piezoelectric actuators inherently suffer from nonlinear characteristics such as hysteresis and creep effects which need to be addressed by appropriate control strategies. The operator-based modified Prandtl-Ishlinksii (mPI) approach does not only model hysteresis effects with asymmetries and creep effects but also provides an analytical solution for its inverse model. Online feedforward compensation of the aforementioned nonlinear effects can be realized by using this inverse model and an additional weight adaptation. In this paper, online compensation via the mPI model is for the first time applied to a system with more than one degree of freedom (DOF). For validation, two coupled trajectories in the X-Y plane are generated which are then implemented on a commercial micro-positioning unit driven by piezoelectric actuators.

Implementing an image based control algorithm for an optomechanical image derotator

B. Altmann, C. Pape (Leibniz Universität Hannover), E. Reithmeier (Leibniz Universität Hannover) 18:10

Rotating components can be found in a wide range of mechanical engineering applications. To study the dynamic behavior of rotating machine components during operation, metrological investigations are necessary. Hence, it can be verified whether demands in performance, safety and efficiency are met. Such measurements are often correlated with major challenges. Contact sensors, for example, influence the system due to their invasive mode of operation. Additionally, the signal transmission via telemetry is complicated due to the movement of the object.

Those disadvantages can be avoided by using non-contact sensors. However, the main problem lies in the investigation of fast rotating objects from a non-rotating measurement system. A solution is provided by an optomechanical image derotator. In generating a stationary image of the rotating object it can be used flexibly in a wide range of metrological tasks. Accordingly, the derotator can be combined with different measurement instruments to perform for example laser vibrometry or thermography as well as image acquisition with a common high-speed camera when its solely use would result in motion blur.

The most important task, concerning the image derotator, lies in adjusting the speed of the derotator with the speed of the measurement object which is constantly changing. If this condition is met, stationary images are enabled by multiple reflections of the object by a rotating mirror assembly inside the derotator. Consequently, accurate and robust information about the object has to be provided constantly. In all current approaches the velocity of the measurement object is investigated by a speed sensor (e.g. a rotary encoder). Nevertheless, only few measurement objects are equipped with such a sensor. This limits the field of application of the image derotator.

In this work a solution is provided by using a high speed camera to generate a feedback source for a control algorithm by tracking the deviation of the measurement object's position. Image processing algorithms are utilized to extract the position of a marker

placed on the measurement object. The marker is segmented from the background so that the relevant information can be extracted and eventually the position of the measurement object can be evaluated from the image data. The so determined control deviation is passed to a controller of the derotator to track the measurement object. By doing this, the purpose of the image based control algorithm is proven. Conclusively, limitations concerning the computation time of the image processing algorithm and therefore of the control algorithm are analyzed and compared for different sampling times of the feedback control system.

S 20 : Dynamics and control

Thursday 14:00 - 16:00 Coudraystr. 11C, Lecture hall 1
Chair: Marleen Stieler (Universität Bayreuth)

HJB-approximations for bilinear control systems with application to the Fokker-Planck equation

T. Breiten (University of Graz), K. Kunisch, L. Pfeiffer 14:00

The probability distribution function of a dragged Brownian particle can be characterized by the Fokker-Planck equation. By means of an optical tweezer, interaction with the particle is possible and leads to a bilinear control system. An optimal feedback law requires solving the Hamilton-Jacobi-Bellman equation, a nonlinear PDE of the dimension of the state space. On the other hand, approximations based on a Taylor series lead to highly structured tensorized linear systems. By means of well-known techniques from tensor calculus, these systems can be efficiently solved even for large-scale dynamical systems. Theoretical and numerical aspects of the resulting feedback law are presented for the Fokker-Planck equation.

Active Impedance Matching in Slender Continua via a Special PID Controller

L. Krumm (Technische Universität Hamburg), E. Kreuzer (Technische Universität Hamburg) 14:20

The concept of impedance matching is well known in electrical engineering and can be applied in mechanical engineering as well. Systems of significant length, which have a relatively low stiffness and should not be treated as a rigid body are typical candidates for the application of impedance matching.
Impedance matching imposes a special boundary condition. In general, at the boundary of a slender mechanical system, waves are partially reflected. The goal of impedance matching is to minimize those wave reflections and to transmit the wave motion to the vicinity. In this paper, it is shown that the impedance matching approach has a great potential of damping vibrations and that a simple PID controller can be used to implement an active version.

Construction of a Lyapunov functional for a class of controlled population balance models

A. Zuyev (Max Planck Institute for Dynamics of Complex Technical Systems), A. Kienle (Max Planck Institute for Dynamics of Complex Technical Systems), P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems) 14:40

Consider a general population balance equation with one spatial variable:

$$\frac{\partial n}{\partial t} + \tilde{G}(n,x)\frac{\partial n}{\partial x} = \tilde{F}(n,x)v, \quad x \in [0,\ell],\ v \in \mathbb{R}, \tag{6.18}$$

where $n = n(x,t)$ describes the distribution of particles of size x at time $t \geq 0$, v is the control, $\tilde{G}(n,x)$ and $\tilde{F}(n,x)$ are given functions. This class of differential equations is used, in particular, for the mathematical modeling of granulation and crystallization processes [2, 3]. If $n = n_d(x)$ is a steady-state solution of the above equation with some constant control $v = v_d$, then by substituting $n(x,t) = n_d(x) + w(x,t)$ and $v = v_d + u$ into (6.18), we obtain:

$$\frac{\partial w}{\partial t} + G(w,x)\frac{\partial w}{\partial x} = F(w,x)u + U(w,x), \tag{6.19}$$

with $G(w,x) = \tilde{G}(w+n_d,x)$, $F(w,x) = \tilde{F}(w+n_d,x)$, and $U(w,x) = Fv_d - G\frac{dn_d}{dx}$. We also assume that the boundary condition $w(0,t) = 0$ holds. In contrast to the discrepancy based approach of the paper [2], dealing with the partial stability problem for the solution $n = n_d$, we focus here on the construction of a positive definite functional $V(w)$ such that its time derivative $\dot{V}(w)$ along the trajectories of (6.19) is non-positive under a suitable choice of the control $u = k(w(\cdot,t))$, and $\dot{V}(w(\cdot,t)) = 0$ only for $w(\cdot,t) = 0$. Such Lyapunov functionals are called strict [1]. *In this work, we show that a strict Lyapunov functional for (6.19) may be (locally) defined in the form*

$$V = \int_0^\ell \rho(x)w^2(x,t)dx, \tag{6.20}$$

if the function $\rho(x) > 0$ satisfies the following differential inequality:

$$\frac{d}{dx}\big(\rho(x)G(0,x)\big) + 2\rho(x)U(0,x) \leq -h(x)\rho(x) \quad \textit{with some } h(x) > 0,\ x \in [0,\ell]. \tag{6.21}$$

We also discuss possible extensions of this approach for the construction of strict Lyapunov functionals in the weighted Sobolev spaces with application to the class of 2×2-hyperbolic systems describing preferential crystallization processes [3].

[1] G. Bastin and J.-M. Coron, *Stability and Boundary Stabilization of 1-D Hyperbolic Systems*, Springer (2016).

[2] S. Palis and A. Kienle, *Discrepancy based control of particulate processes*, J. Process Control, 24 (2014), pp. 33-46.

[3] S. Qamar, A. Ashfaq, I. Angelov, M.P. Elsner, G. Warnecke, and A. Seidel-Morgenstern, *Numerical solutions of population balance models in preferential crystallization*, Chem. Eng. Sci., 63 (2008), pp. 1342–1352.

Approximation and implementation of transformation based feedback-laws for distributed parameter systems

S. Ecklebe (Technische Universität Dresden, Fak. Elektro- und Informationstechnik), M. Riesmeier (UMIT – Private University of Health Sciences, Medical Informatics and Technology), F. Woittennek (UMIT – Private University of Health Sciences, Medical Informatics and Technology) 15:00

This talk presents an approach to the efficient numerical approximation and implementation of state feedback for linear distributed parameter systems. The control laws considered may originate from backstepping [1] and flatness based [2] design methods. They are, therefore, directly based on the underlying distributed parameter systems and, as a consequence, of infinite dimensional nature. These methods typically result in feedback laws of the form

$$u(t) = (\mathrm{P}x)(t) + (\mathrm{K}x)(t)\,, \tag{6.22}$$

where P denotes an unbounded operator, for example containing boundary evaluations of the distributed system variables. In contrast, the operator K is a bounded linear functional on the state space, incorporating expressions like integral operators arising from the backstepping transformation. While the unbounded part can often be realized using measurements on the system's boundary, determining the bounded part is frequently linked to tremendous computational effort.
Within the present contribution an approach for the approximation of this unbounded part of the feedback law is presented which, moreover, may essentially simplify the controller design itself. This is achieved by the projection of the system state on an appropriately chosen finite dimensional subspace of the state-space. The choice of this space as well as the implementation of the derived controller is discussed for both, the general case and an particular example. For the implementation and validation of the obtained approximated controllers the python based software toolbox PyInduct [3] is introduced.

[1] Krstic, M. and Smyshlyaev, A. (2008). Boundary Control of Pdes: A Course on Backstepping Designs. Society for Industrial and Applied Mathematics Philadelphia, PA, USA.

[2] Woittennek, F. (2013). Flatness based feedback design for hyperbolic distributed parameter systems with spatially varying coefficients. In *Proc. 1. IFAC Workshop on Control Systems Modelled by Partial Differential Equations*. Paris.

[3] Ecklebe, S. and Riesmeier, M. (2016). *PyInduct Documentation*. URL `https://pyinduct.readthedocs.org`. March 4, 2017.

An operator based notation of the Lagrange equations for systems with non-material boundary conditions

A. Franze (Institute of Mechanics and Shell Structures, TU Dresden) 15:20

Problems with non-material boundary conditions are very important in many applications of continuum mechanics: for example rolling contact, calenders, breaking disks, band saws and belts. This paper deals with the Lagrange-equation for non-material boundary conditions. Such boundary conditions can be described by non-material control volumes that cannot be assigned for one and only one set of particles over time. To define these volumes, a fictitious body is used. Within the scope of this paper several configurations are introduced for the definition of the location of the original and fictitious particles. With the help of the used operator notation it is possible to demonstrate a consistent representation of derivative operators and assign operators as well as entities to their configurations.
On this basis, the Lagrange-equation is derived for material and non-material control volumes inthe eulerian and lagrangian representation. These equations are illustrated and verified with demonstrative examples. Furthermore, the verification of the eulerian and lagrangiandescription of the control volume is achieved.

[1] A. Franze, B.W. Zastrau, On the Transverse Vibrations of a String Segment Between Two Supports Moving Axially Along a String of Infinite Length, Proceedings in Applied Mathematics and Mechanics, 10(1), 237-238 (2010)

[2] A. Franze, B.W. Zastrau, Analytical solution for the one-dimensional wave equation with non-material boundary conditions, In: Selected dynamical problems in mechanical systems – theory and applications in transport (2014)

Some remarks on linear systems

F. Woittennek (UMIT – Private University of Health Sciences, Medical Informatics and Technology) 15:40

Linear Systems with lumped and distributed parameters are considered. For this class of models the talk aims for a notion of linear systems that is compatible with both, the usual notion of a linear dynamical system defined on a finite or infinite dimensional state space (cf. [3]) and, moreover, with the elegant trajectorian or behavioral definition proposed by Willems (cf. [2, 1]). As a consequence the starting point is mainly the behavioral definition viewing a system as the set of its solutions or trajectories. In order to avoid the necessity of choosing particular function spaces the solutions are defined on, only some basic structural properties of the solution spaces are required. These properties, basically, allow for the definition of time-shifts as required for the notion of time-invariance. Naturally, two time-invariant systems are called equivalent if their solution sets are isomorphic by means of a shift-invariant map. This allows for a straitforward definition of the notions of inputs or flatness. Moreover, some well known facts as the equivalence of systems described by hyperbolic p.d.e. and systems described by delay-differential equations smoothly integrate within the proposed framework. Furthermore, based on these basic definitions, established notions as state-space and state may be

introduced in an very convenient way. While the definitions slightly differ from those used within the standard behavioral approach, they may be immediately seen to be compatible with the established state-space approach to linear systems based on semi-groups. Apart from these and very much inspired by the theory of flat (finite dimensional) systems several other interesting notions as (quasi-)static or endogenous feedback may be given within the proposed framework.

[1] Polderman, J. W. and J. C. Willems: *Introduction to Mathematical System Theory: A Behavioral Approach*. Springer-Verlag, New York, 1998.

[2] Willems, J. C.: *Paradigms and puzzles in the theory of dynamical systems*. IEEE Trans. Automat. Control, 36:259–294, 1991.

[3] Curtain, R. F. and Zwart, H.: *An Introduction to Infinite-dimensional Linear Systems Theory*. Springer-Verlag, New York, 1995.

S 20 : Dynamics and control

Thursday 16:30 - 18:30 Coudraystr. 11C, Lecture hall 1
Chair: Tobias Breiten (Universität Graz)

Hankel-Norm Approximation of Descriptor Systems

S. Werner (Max Planck Institute for Dynamics of Complex Technical Systems), P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems) 16:30

The aim of model reduction is to approximate the original system by a cheap-to-evaluate surrogate. Most of the known methods were developed for the case of standard linear continuous-time systems

$$\begin{aligned} \dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{aligned} \tag{6.23}$$

with system matrices $A \in \mathbb{R}^{n\times n}$, $B \in \mathbb{R}^{n\times m}$, $C \in \mathbb{R}^{p\times n}$, and $D \in \mathbb{R}^{p\times m}$. Since model reduction methods produce approximations, an often mentioned problem is the construction of a reduced-order model which minimizes the approximation error in a certain system norm. The Hankel-norm approximation is such a method. Here the reduced-order model minimizes the approximation error in the Hankel-norm

$$||G||_H = \sup_{u_-\in\mathcal{L}_2} \frac{||y_+||_{\mathcal{L}_2}}{||u_-||_{\mathcal{L}_2}},$$

with past inputs u_- and future outputs y_+. Based on the work of Adamjan, Arov, and Krein, a Hankel-norm approximation method for standard systems (6.23) was developed by Glover in [1].

But the modeling of many applications, like mechanical systems and fluid dynamics, results in descriptor systems

$$\begin{aligned} E\dot{x}(t) &= Ax(t) + Bu(t), \\ y(t) &= Cx(t) + Du(t), \end{aligned} \tag{6.24}$$

with a singular $E \in \mathbb{R}^{n\times n}$ matrix. One approach for the computation of the generalized Hankel-norm approximation of (6.24) was given in [2]. Therefor, the Weierstrass canonical form of the matrix pencil $\lambda E - A$ in (6.24) is computed and explicit construction formulas for the resulting subsystems are used. The main problem of this approach is the numerically unstable and costly computation of the Weierstrass canonical form. This problem makes this approach hardly applicable to practical examples, especially the instability may cause problems in the later transformations of the Hankel-norm approximation.
A much more efficient and stable method results from a refinement of the generalized balanced truncation square-root method introduced by Stykel in [3]. The resulting generalized Hankel-norm approximation method can be applied to a broad field of practical examples, including the case of sparse system matrices.

[1] K. Glover. All optimal Hankel-norm approximations of linear multivariable systems and their L$^\infty$-error norms. *Internat. J. Control*, 39(6):1115–1193, 1984.

[2] X. Cao, M. B. Saltik, and S. Weiland. Hankel model reduction for descriptor systems. In *2015 54th IEEE Conference on Decision and Control (CDC)*, pages 4668–4673, December 2015.

[3] T. Stykel. Gramian-based model reduction for descriptor systems. *Math. Control Signals Systems*, 16(4):297–319, 2004.

Model approximation with multiplicative isometric operators in H_2

C. Zimmer (TU Berlin), I. Pontes Duff (MPI Magdeburg) 16:50

The mathematical description of physical, chemical, or biological processes often leads to control problems with a large number of degrees of freedom and therefore to systems with high computational costs. The aim of model order reduction is on the one hand to lower the computational time as well as the complexity of the model, and on the other hand to maintain the input-output-behavior. One approach for this task is to search for a linear time-invariant system (LTI-system) with a minimal error in the Hardy-space $\mathcal{H}_2$.
In this talk we will investigate the approximation behavior of LTI-systems with additional multiplicative isometric operators of $\mathcal{H}_2$, e.g., the operators of input-output-delays in the time domain. The advantage of this approach is that it maintains the energy of impulse responses of the reduced order model and leads to a bigger class of possible models for the approximation at the same time. For this class we will derive a representation of

the error, calculate optimality conditions and show numerical examples with parameter dependent operators.

H_2-Optimal Model Order Reduction for Second Order Systems

P. Benner (Max Planck Institute for Dynamics of Complex Technical Systems), S. Grundel, P. Mlinarić (Max-Planck-Institut für Dynamik komplexer technischer Systeme) 17:10

The Two Sided Iteration Algorithm (TSIA) is a method for $\mathcal{H}_2$-optimal model order reduction of linear time-invariant systems, based on necessary conditions for $\mathcal{H}_2$-optimality in matrix equation form (Wilson conditions). When TSIA is applied to a second order system, the resulting reduced model will not necessarily have second order structure. Preserving the second order structure might be desirable in applications, since it gives a better physical description of the underlying system. Following the derivation of Wilson conditions, we find the necessary conditions for a second order system of reduced order to be $\mathcal{H}_2$-optimal. From this, we propose an algorithm, analogous to TSIA, for structure preserving $\mathcal{H}_2$-optimal model order reduction of second order systems. We demonstrate it on a mass-damper-spring system example.

Modeling and evaluation of cyber-physical systems in civil engineering

D. Legatiuk (Bauhaus-Universität Weimar), K. Dragos (Bauhaus-Universität Weimar), K. Smarsly (Bauhaus-Universität Weimar) 17:30

A cyber-physical system (CPS) is a coupled system integrating computing, networking, and physical processes. Through actuation, cyber-physical systems control the physical processes, usually with feedback loops, where the physical processes affect computing and networking processes, and vice versa. In civil engineering, the most common fields of CPS applications are structural health monitoring (SHM) and structural control. The task of such a coupled system is the assessment of a structure based on (i) collected measurement data and (ii) a corresponding model. However, for an accurate and precise assessment of a structure, the CPS itself must be modeled and evaluated. In this paper, a modeling and evaluation approach is proposed, in which each part of a CPS is evaluated individually. In addition, the couplings between CPS models and SHM system are considered. In this study, the conceptual approach is demonstrated for modeling and evaluation of CPS in civil engineering. The evaluation is based on an abstract approach allowing a discussion of a principle (i.e. general) model structure of a CPS, identifying critical issues to be studied in more detail in future research.

Modeling a heavy rope using redundant coordinates

D. Gerbet (Universität des Saarlandes), J. Rudolph 17:50

The Lagrange formalism is an elegant method for modeling mechanical systems. It requires, however, that the potential energy and the kinetic coenergy be written in terms of independent coordinates. For some systems, finding a set of independent coordinates

such that no singular configurations occur is challenging or even impossible. Thus, a description using redundant coordinates may be preferred. In [1] a generalization of the Lagrange formalism is presented that allows for a description of the mechanical problem using independent velocities but redundant coordinates. The latter are constrained to a manifold by nonlinear algebraic equations. In addition to the avoidance of singular configurations, this method lends itself to the connection of subsystems by algebraic constraints, thus avoiding the labour associated with finding new independent coordinates for the composite system.
The generalized Lagrange formalism is also applicable to systems with distributed parameters. This will be illustrated through an example of a heavy rope. The resulting mathematical model for the rope in three-dimensional space is singularity-free, at the expense of redundant coordinates constrained by nonlinear equations.

[1] M. Konz and J. Rudolph. Beispiele für einen direkten Zugang zu einer globalen, energiebasierten Modellbildung und Regelung von Starrkörpersystemen. at – Automatisierungstechnik 2016; 64(2):96–109

Zeno phenomenon in hybrid dynamical systems

S. Dashkovskiy (University of Würzburg), P. Feketa (University of Applied Sciences Erfurt) 18:10

In some applications one has to deal with a combination of continuous and discontinuous behaviour in one model. Several modelling frameworks (hybrid, impulsive and other systems) exist for such dynamical systems. In all of these models the Zeno type solutions (infinite number of jumps on a finite time interval) can appear which leads to a common problem in all these frameworks: such solutions are defined only up to the Zeno time point, which is a finite number. This phenomenon can lead to unnatural loss of stability of equilibriums and the emergence of unexpected and meaningless solutions in case of interconnected systems. Many works are devoted to the question of prolongation of such solutions, however there exist no unified or commonly accepted prolongation method. In our talk we are interested in the asymptotic stability properties for this kind of solutions, which is also not completely solved in the literature. We will provide an approach for the prolongation of solutions over the Zeno time and we will present a novel concept of stability that characterizes long-term asymptotic behaviour of solutions and supply it with a constructive Lyapunov-like theorem for its verification. Our results are in particular suitable for the investigation of the stability properties of interconnected hybrid systems.

S 21: Mathematical signal and image processing

Organizers: Gabriele Steidl
Jan Lellmann (Universität zu Lübeck)

S 21 : Mathematical signal and image processing

Tuesday 14:00 - 16:00 Weimar hall, Seminar room 1

Harmonic Mean Iteratively Reweighted Least Squares for Low-Rank Matrix Recovery with Superlinear Convergence

J. Sigl 14:00

We propose a new Iteratively Reweighted Least Squares (IRLS) algorithm for the problem of recovering a low-rank matrix from incomplete linear observations, named Harmonic Mean Iteratively Reweighted Least Squares (`HM-IRLS`). It introduces enhanced, so-called *harmonic mean weight matrices*, which lead to an improved minimization of the nonconvex Schatten-p functional compared to previous IRLS approaches to the problem. We extend the theoretical guarantees of existing low-rank IRLS algorithms, both general ones and those based on *null space properties* of the linear measurement operator, to `HM-IRLS`. Furthermore, we show that `HM-IRLS` exhibits a *local superlinear convergence rate* (of order $2 - p$) in case of convergence to a low-rank matrix. Note that for the empirically most promising choices of very small Schatten-p parameters $p \ll 1$, the convergence rate is *almost quadratic*. We verify the theoretically predicted superlinear convergence rate in our experiments accurately for the important case of matrix completion although our guarantees only partially apply to this model. We stress that a superlinear rate of convergence is *unprecedented both in theory and practice* for any low rank matrix recovery algorithm in the literature. Moreover, we conduct extensive numerical experiments comparing the measurement sample complexity of `HM-IRLS` with related algorithms as well as with algorithms based on different concepts, focussing on the matrix completion setting. We observe that surprisingly, `HM-IRLS` only needs very few given entries (*very close to the information theoretical lower bound*) to complete low rank matrices with high empirical probability, *fewer than all the state-of-the-art algorithms* we included in our experiments. It is remarkable as well, that convergence to nonglobal minima is not an issue for our algorithm despite the strong nonconvexity of the problem for $p \ll 1$.

Analysis of the geometry of edges by the Taylorlet transform

T. Fink 14:20

In numerous fields of image analysis, analyzing the precise geometry of edges is a crucial task. To this end, various methods for the detection of some of their geometric quantities have already been developed. Among them the continuous shearlet transform offers a

micro-analytic possibility to resolve the wavefront set of a function and thus to identify the position and orientation of an edge through the transform's decay rate at fine scales. In order to additionally extract higher order geometric information of edges such as its curvature, we consider the Taylorlet transform which is an extension of the continuous shearlet transform and uses nonlinear shearings. This transform exhibits an adjustable, polynomially fast decay rate at fine scales for the case that not all of its shearing parameters equal the corresponding geometric quantities of the edge and thus allows for their reliable detection.

Variational methods for phase or orientation data

M. Storath (Universität Heidelberg) 14:40

We consider variational methods for signals and images which take their values on the unit circle S^1 (or $\mathbb{T}$). Circle-valued data appear naturally as orientation data, for example in the rotation of the bacterial flagellar motor, as wind directions, or when considering the orientation component of planar flow fields. Also phase signals which are defined modulo 2π are circle-valued, for example interferometric synthetic aperture radar images. As the unit circle is not convex, variational regularization methods lead to challenging optimization problems for such data. Even total variation (TV) regularization, given by

$$u^* = \arg\min_{u\in\mathbb{T}^{m\times n}} \gamma \sum_{ij} d(u_{ij}, u_{i,j+1}) + \gamma \sum_{ij} d(u_{ij}, u_{i+1,j}) + \sum_{ij} d(u_{ij}, f_{ij})$$

where $f \in \mathbb{T}^{m\times n}$ is a circle-valued image and d denotes the arc distance metric, becomes a non-convex problem. In the talk, we present new minimization methods for variational problems such as TV or Potts regularization for circle-valued data. We provide exact solvers for univariate data and approximative strategies for higher dimensional data. The presented methods were developed in joint works with Laurent Demaret, Michael Unser, and Andreas Weinmann [1, 2, 3, 4].

[1] A. Weinmann, L. Demaret, M. Storath. *Total variation regularization for manifold-valued data.* SIAM Journal on Imaging Sciences, 7(4):2226-2257, 2014

[2] M. Storath, A. Weinmann, M. Unser. *Exact algorithms for L1-TV regularization of real-valued or circle-valued signals.* SIAM Journal on Scientific Computing, 38(1):A614-A630, 2016

[3] A. Weinmann, L. Demaret, M. Storath. *Mumford-Shah and Potts regularization for manifold-valued data.* Journal of Mathematical Imaging and Vision, 55(3):428-445, 2016

[4] M. Storath, A. Weinmann, M. Unser. *Jump-penalized least absolute values estimation of scalar or circle-valued signals.* Information and Inference, to appear

Multiscale statistical regularisation for inverse problems in imaging

M. Grasmair (NTNU) 15:00

For the solution of inverse problems in imaging, it is often desirable to use locally adaptive methods where the amount of regularisation depends on the local structures of the image to be reconstructed. In this talk, we will present such a method, which is based on a multi-scale analysis of the residual. Assuming that the measurement errors are independent and identically normally distributed, the residuals should ideally look like a typical sample of an i.i.d. Gaussian random variable. This can be exploited by looking at the behaviour of local sums of the residual. If the residual actually is i.i.d. Gaussian, then these local sums can be expected to be relatively small. On the other hand, the local sums will be large, if the residual still contains parts of the true image.
In order to exploit the prior knowledge of the noise, we propose to use a variational regularisation method. The method uses non-quadratic Tikhonov regularisation with a Sobolev (or total variation) based regularisation term and a data fidelity term involving the maximum of weighted local means of the residual. Assuming certain source conditions, we will derive convergence rates in expectation for the reconstruction as the number of measurements tends to infinity. Additionally, we will briefly discuss the optimality of these convergence rates and provide cases where they are - up to a logarithmic term - asymptotically optimal.

Multiframe Motion Coupling for Video Super Resolution

H. Dirks (Westfälische Wilhelms-Universität Münster), J. Geiping (University of Siegen), D. Cremers (Technical University of Munich), M. Möller (University of Siegen) 15:20

The idea of video super resolution is to use the temporal information of seeing a scene from many slightly different viewpoints in the successive frames of a video to enhance the overall resolution and quality of each frame. In this talk we will present a novel variational approach for the video super resolution problem. Instead of coupling each unknown high resolution frame with several of the observed low resolution frames, we propose to couple the high resolution frames directly and solve for the entire super-resolved video in a single joint optimization approach. As a consequence, the number of required motion estimation problems grows linearly in the number of frames, opposed to a quadratic growth of classical methods. In addition, we use infimal convolution regularization to automatically determine the reliability of the motion information and reweight the regularization locally. We demonstrate that our approach yields temporally consistent high resolution results and even is competitive with learning based approaches that require a significant amount of training data.

Error analysis for filtered back projection reconstructions in fractional Sobolev spaces

M. Beckmann (University of Hamburg), A. Iske (University of Hamburg) 15:40

The term filtered back projection (FBP) refers to a well-known and commonly used reconstruction technique in computerized tomography, which allows us to reconstruct a bivariate function from its given Radon samples. The FBP formula, however, is

numerically unstable and suitable low-pass filters of finite bandwidth and with a compactly supported window function are employed to make the reconstruction by FBP less sensitive to noise.
The objective of this talk is to analyse the inherent reconstruction error which is incurred by the application of the chosen low-pass filter. To this end, we present error estimates in Sobolev spaces of fractional order. The obtained error bounds depend on the bandwidth of the low-pass filter, the flatness of the filter's window function at the origin as well as the difference between the smoothness of the target function and the order of the considered Sobolev norm. Further, we show convergence for the approximate FBP reconstruction in the treated Sobolev norms along with asymptotic convergence rates, where the filter's bandwidth goes to infinity.

S 21 : Mathematical signal and image processing

Tuesday 16:30 - 18:30 Weimar hall, Seminar room 1

A new supervised NMF algorithm

D. Lachmund (University of Bremen), T. Boskamp (University of Bremen), P. Fernsel (University of Bremen), P. Maaß (University of Bremen) 16:30

Hyperspectral data often can be modelled as a superposition of unknown basic patterns. In case an additional non-negativity constraint is desired a discrete variational formulation leads to well known NMF functionals (Non-negative Matrix Factorization). Following an algorithmic MM framework (Majorization-Minimization) multiplicative update rules can be deduced for a variety of different discrepancy terms and extensions [1, 2, 3].
In general the resulting factorizations offer insight into underlying processes and serve as a natural feature extraction. However, by following the described procedure usually only the most prominent features can be found, partly due to the often required dimensionality reduction. In the training phase of classification pipelines additional label information is available, and globally rather subtle features with strong discriminating ability are in the focus of interest. Recently first efforts have been made to utilize this label information to fine-tune existing NMF models, thereby effectively turning the unsupervised feature extraction into a supervised one [4, 5, 6].
In this work we introduce a new supervised NMF model and deduce alternating update rules for the minimization. Applications on mass spectrometry imaging data will serve as a demonstration of feasibility and effectiveness.

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[2] Févotte, Cédric. "Majorization-minimization algorithm for smooth Itakura-Saito nonnegative matrix factorization." *Acoustics, Speech and Signal Processing (ICASSP), 2011 IEEE International Conference on.* IEEE, 2011.

[3] Wang, Yu-Xiong, and Yu-Jin Zhang. "Nonnegative matrix factorization: A comprehensive review." *IEEE Transactions on Knowledge and Data Engineering* 25.6 (2013): 1336-1353.

[4] Lee, Soo-Young, Hyun-Ah Song, and Shun-ichi Amari. "A new discriminant NMF algorithm and its application to the extraction of subtle emotional differences in speech." *Cognitive neurodynamics* 6.6 (2012): 525-535.

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Analytical aspects of spatially adapted total variation regularisation

K. Papafitsoros (Weierstrass Institute for Applied Analysis and Stochastics), M. Hintermüller, C. Rautenberg, M. Holler 16:50

Spatially adapted regularisation in image reconstruction has been used in order to preserve details like texture and other highly oscillating features that are naturally present in the image. The idea is to apply regularisation of different strength in different parts of the image by spatially varying the regularisation parameters. In this talk, starting from the case of continuous weight functions, we will present analytical results regarding the effect of the spatially varying parameters to the structure of solutions of weighted total variation regularisation. Moreover, we will set up a proper analytical framework regarding a weighted total variation functional defined for a wide class of weights tailored for use in inverse problems.

Applications of the graph p-Laplacian in image processing

D. Tenbrinck (WWU Münster), A. Elmoataz (Université de Caen Normandie) 17:10

Graph-based methods are a promising tool, which can be applied to images modeled as a graph. This graph model allows to exploit both local as well as nonlocal relationships in the data for image processing. A recent trend in the literature is to translate well-studied variational problems and PDEs to finite weighted graphs and study their characteristics in this discrete setting. In this talk we give a short introduction to the concept of mimicking partial difference equations on graphs. As particular example we discuss a family of partial difference operators on graphs known as the graph p-Laplacian. We demonstrate the potential of these operators for a variety of different tasks in image and point cloud processing, such as filtering, segmentation, clustering, and inpainting.
Joint work with A. Elmoataz, Université de Caen, France

Graph Methods for Manifold-valued Data

R. Bergmann (TU Kaiserslautern), D. Tenbrinck (University of Münster) 17:30

Due to recent technological advances in the development of modern sensors new imaging modalities have emerged for which the acquired data values are given on a Riemannian manifold. This is the case, e.g., when dealing with Interferometric Synthetic Aperture Radar (InSAR) data consisting of phase values or data obtained in Diffusion Tensor

Magnetic Resonance Imaging (DT-MRI), where each measurement is a positive definite matrix of size 3x3. Furthermore, the data might not be given on a rectangular pixel grid but on a surface or a manifold itself. For these emerging imaging fields novel image processing techniques have to be developed and adapted.
In this talk we present a framework for processing discrete manifold-valued data, for which the underlying (sampling) topology is modeled by a graph. We introduce the notion of a manifold-valued derivative on a graph and based on this deduce a family of manifold-valued graph p-Laplacian operators. We propose an efficient numerical scheme to compute a solution to the corresponding parabolic PDEs and apply this algorithm to different manifold-valued data, illustrating the diversity and flexibility of the proposed framework.
This is joint work with Daniel Tenbrinck, University of Münster.

Unbalanced Optimal Transport: A Practical Guide

B. Schmitzer (WWU Münster) 17:50

Optimal transport induces a geometrically meaningful metric on the space of histograms and probability measures and is a powerful tool for image and data analysis. With the evolution of efficient numerical methods it is becoming increasingly popular. However, in many models the assumption that all measures have unit mass and that mass is exactly preserved locally are too restrictive, for instance in biochemical growth processes. Hence, in recent years, 'unbalanced' transport problems, that allow creation or annihilation of mass during transport, have received increased attention. In this talk we present several formulations for such problems, efficient numerical methods and illustrate applications and advantages of unbalanced metrics.
This is joint work with Lénaïc Chizat, Gabriel Peyré, François-Xavier Vialard and Benedikt Wirth.

An approach to image reconstruction based on partially ordered spaces and applications in diffusion tensor imaging

Y. Korolev (Universität zu Lübeck) 18:10

Image reconstruction often relies on the solution of a (typically ill-posed) inverse problem. To guarantee numerical stability of the inversion, regularization needs to be applied, which requires the understanding of the errors (noise) in the data and, possibly, in the forward model. In the context of variational regularization, different fidelity functionals have been proposed to model different types of noise, e.g., the L_2-norm for Gaussian noise or the L_1-norm for salt-and-pepper noise. Partial order provides an alternative approach to noise modelling which does not assume a particular distribution of the noise and can be useful in situations when exact noise modelling is challenging. This talk will introduce inverse problems in functional spaces with partial order and present numerical results in diffusion tensor imaging (DTI), where exact noise modelling involves Rician noise and the non-linear Stejskal-Tanner equation. Partial order allows to avoid complicated noise models by providing a simple and computationally efficient approximation of the fidelity.

S 21 : Mathematical signal and image processing

Wednesday 16:30 - 18:30 Coudraystr. 13B, 2nd floor, Room 210

A geometric reasoning for Tyler standardisation of projective shapes

T. Hotz (TU Ilmenau) 16:30

Projective shapes encode the information that can be extracted from scenes based on uncalibrated camera views. To obtain a space of projective shapes amenable to statistical analyses, Kent and Mardia (Biometrika, 2012) proposed to consider pre-shapes which are Tyler standardised, i.e. the configuration's moment of inertia matrix is a multiple of the identity matrix while the landmarks have unit norm. Using a Veronese-Whitney embedding, only a discrete group action is left. We show that this standardisation can be given a natural, geometric interpretation by computing the infinitesimal generators of the rescaling as well as the projective group's action on a configuration.

Supervised learning on medical OCT images

A. Breger (University of Vienna) 16:50

Spectral-domain optical coherence tomography (OCT) is nowadays the most frequently used imaging technology in ophthalmology. It provides good visualization of retinal fluid, which is observed in various ocular disorders associated with vision loss and is related to disease severity. Here we will present a fully automated image analysis pipeline tailored to fluid quantification in OCT images based on dimension reduction techniques with a fast learning part and low memory needs. We work with 38 OCT volumes, each containing 128 cross-sectional images (B-scans), as well as respective binary pixel wise ground truth manually annotated by retina specialists at the Vienna Reading Center (VRC). The pipeline consists of mainly 5 sub-steps including local and global feature selection, pre-segmentation via energy minimization and finally supervised learning of a threshold value. Overall it is easy to implement, requires only few training data and yields good visualization and fluid quantification.

This is joint work with

Hrvoje Bogunovic *(Department of Ophthalmology, Medical University of Vienna)*
Bianca S. Gerendas *(Vienna Reading Center, Department of Ophthalmology, Medical University of Vienna)*
Ursula Schmidt-Erfurth *(Department of Ophthalmology, Medical University of Vienna)*
Martin Ehler *(Department of Mathematics, University of Vienna)*

Advances in Robust Blind Variational Image Deconvolution

M. Welk (UMIT) 17:10

In work by Liu et al. (2014), a novel regulariser for variational blind image deconvolution was proposed that is based on the convolution spectrum of a blurred image. In a recent

contribution coauthored by the author of this talk, this regulariser was embedded into a robust deconvolution framework. In this talk, further improvements of the latter framework will be discussed, which address the issue of non-matching data terms for the alternating estimation of point-spread function and image. Moreover, problems of evaluation of the blind deconvolution framework by error measures are addressed.

Optimal Numbers of Edges in Deep Neural Networks

G. Kutyniok (Technische Universität Berlin), P. Grohs (Universität Wien), P. Petersen (Technische Universität Berlin) 17:30

Despite the outstanding success of deep neural networks in real-world applications, most of the related research is empirically driven and a mathematical foundation is almost completely missing. One central task of a neural network is to approximate a function, which for instance encodes a classification task. In this talk, we will be concerned with the question, how well a function can be approximated by a sparse neural network. Using methods from approximation theory and applied harmonic analysis, we will prove a fundamental lower bound on this sparsity if certain approximation properties are required. Moreover, we will demonstrate that this lower bound can be attained.

A Region Based Easy Path Wavelet Transform for Sparse Image Representation

R. Budinich 17:50

In [1] G. Plonka proposed an innovative method for sparse image representation: successively finding a suitable path in the image (i.e. reducing it to a one-dimensional signal) and applying one level of a one dimensional wavelet transform. This yields a sparse representation which behaves better than the typical tensor product wavelet transform. However there are adaptivity costs: for each level one has to store the path, i.e. a permutation of the pixel points.

We propose a variation on this method, which consists in first segmenting the image into regions, then successively for every level finding in each region a path (in some canonical manner, not depending on the pixel values) and applying a one-dimensional wavelet transform to it. This method is particularly well-suited to encode a part of the image (region of interest) with higher quality than the rest. We will discuss various details of this approach and present some numerical experiments.

Multiscale Image Representations for Ultrasound Visual Servoing

R. Reisenhofer (Universität Bremen), L. Duflot (INRIA Rennes-Bretagne Atlantique), B. Tamadazte (FEMTO-ST), N. Andreff (FEMTO-ST), A. Krupa (INRIA Rennes-Bretagne Atlantique) 18:10

We present a novel approach to visual servoing, in which the feature vector used to guide the visual servoing process is obtained by considering the coefficients of wavelet-

[1] G. Plonka, The easy path wavelet transform: A new adaptive wavelet transform for sparse representation of two-dimensional data, Multiscale Model. Simul. 7 (2009), 1474–1496.

and shearlet-based transforms of the image currently observed by an imaging device, such as an ultrasound probe.

Two- and three-dimensional ultrasound imaging devices are widely used in medicine for non-invasive observations of inner organs. In this context, robotic systems have been developed to automatically compensate for patient movements in order to keep the observed ultrasound image as stable as possible. This is typically achieved by continuously adjusting the position of an ultrasound probe such that the error between a currently observed set of features $\mathbf{s} \in \mathbb{R}^N$ and a desired set of features $\mathbf{s}^* \in \mathbb{R}^N$

$$\mathbf{e} = \mathbf{s} - \mathbf{s}^*,$$

is minimized by applying the Levenberg-Marquardt algorithm

$$\mathbf{v} = -\lambda \left((\mathbf{L_s}^\intercal \mathbf{L_s} + \mu \operatorname{diag}(\mathbf{L_s}^\intercal \mathbf{L_s}) \right)^{-1} \mathbf{L_s}^\intercal \mathbf{e},$$

where the movement of a robot with k degrees of freedom is expressed via the velocity vector $\mathbf{v} \in \mathbb{R}^k$ and $\mathbf{L_s} \in \mathbb{R}^{N \times k}$ denotes a so-called interaction matrix encoding how the observed features $\mathbf{s}$ change with respect to $\mathbf{v}$.

We show how the matrix $\mathbf{L_s}$ corresponding to a shearlet- or wavelet-based feature vector $\mathbf{s}$ can be explicitly computed at a given point in time and present experimental evidence that shearlet- and wavelet-based methods can increase the reliability of visual servoing systems in the presence of external disturbances such as varying lighting conditions.

S 21 : Mathematical signal and image processing

Thursday 14:00 - 16:00 Coudraystr. 13B, 2nd floor, Room 210

Denoising of Image Gradients and Constrained Total Generalized Variation

B. Komander (TU Braunschweig), D. Lorenz (TU Braunschweig) 14:00

In the paper from 2004, Lysaker et. al. [M. Lysaker, S. Osher, X. C. Tai, IEEE Trans. Img. Proc. 13(10) (October 2004) 1345-1357] proposed an image denoising technique in two steps. First, they used a total variation filter in order to smooth normal vectors of the level-sets of a given noisy image. After that, they tried to find a surface to fit these smoothed normal vectors.
In [B. Komander, D. Lorenz, M. Fischer, M. Petz, R. Tutsch, J. Sens. Sens. Syst. (2014) 281-290] a similar idea has been applied for a problem of deflectometric surface measurements, where the measurement device produces approximate point coordinates with additional approximate surface normals. There, due to the measurement process itself the surface normals where of higher magnitude than the point coordinates.
In both cases the resulting optimization problems where highly non-linear. Switching from surface normals to image gradients, however, turns out to lead to a linear problem.

Therefore, we derive a denoising method that used higher order derivative informations which is motivated by the mentioned work on denoising of normal vectors of the image which then are used for better denoising of the image itself. We propose denoising of image gradients which leads to a convex optimization problem.
Furthermore, we show how the denoising of the image gradients and the image itself can be done simultaneously in one optimization problem. It turns out that the resulting problem is similar to total generalized variation denoising, thus shedding more light on the motivation of the total generalized variation penalties. Our approach, however, works with constraints, rather than penalty functionals. As a consequence, there is a natural way to choose one of the parameters of the problems and we motivate a choice rule for the second involved parameter.

Surface Normal Integration by Hyperbolic PDEs

M. Breuß (BTU Cottbus - Senftenberg), M. Bähr (BTU Cottbus - Senftenberg) 14:20

The integration of surface normals is a classic problem in computer vision. We consider hyperbolic partial differential equations for dealing with the task. A thorough numerical investigation of possible model variants is presented that highlights important issues in modelling and numerics. We conclude that hyperbolic models can represent a viable approach to surface normal integration, especially if the domain of integration is non-quadratic.

Finite-Valued Sparse Signals

S. Keiper (TU Berlin), G. Kutyniok (Technische Universität Berlin), D. Lee, G. Pfander 14:40

The need of reconstructing discrete-valued sparse signals from few measurements, that is solving an undetermined system of linear equations, appears frequently in science and engineering. Those signals appear, for example, in error correcting codes as well as massive Multiple-Input Multiple-Output (MIMO) channel and wideband spectrum sensing. A particular example is given by wireless communications, where the transmitted signals are sequences of bits, i.e., with entries in $\{0, 1\}$. Whereas classical compressed sensing algorithms do not incorporate the additional knowledge of the discrete nature of the signal, classical lattice decoding approaches do not utilize sparsity constraints.
In this talk, we present an approach that incorporates a discrete values prior into basis pursuit. In particular, we address finite-valued sparse signals, i.e., sparse signals with entries in a finite alphabet. We will introduce an equivalent null space characterization and show that phase transition takes place earlier than when using the classical basis pursuit approach. We will further discuss robustness of the algorithm and show that the nonnegative case is very different from the bipolar one. One of our findings is that the positioning of the zero in the alphabet - i.e., whether it is a boundary element or not - is crucial.

Box-constrained total variation minimisation

A. Langer 15:00

A good approximation of the original image from an observed image may be obtained by minimising a functional that consists of a data-fidelity term, a regularisation term, and a parameter, which balances data-fidelity and regularisation. Using the total variation as a regularisation term is a rather well understood concept of restoring images while preserving edges and discontinuities. If we have knowledge about the dynamic range in which the original image lies, then it seems natural to incorporate this information (via a box-constraint) into the model. Moreover, it is clear that the minimiser of the considered functional highly depends on the proper choice of the parameter.
In this talk we are wondering whether incorporating a box-constraint into the model really improves the quality of the solution or if it is indeed more a question of the proper choice of the regularisation parameter. Further we propose a semi-smooth Newton method for solving the considered models.

A Dual Ascent Framework for Lagrangean Decomposition of Combinatorial Problems

P. Swoboda, B. Savchynskyy (TU Dresden) 15:20

We propose a general dual ascent framework for Lagrangean decomposition of combinatorial problems. Although methods of this type have shown their efficiency for a number of problems, so far there was no general algorithm applicable to multiple problem types. In this work, we propose such a general algorithm. It depends on several parameters, which can be used to optimize its performance in each particular setting. We demonstrate efficacy of our method on graph matching and multicut problems, where it outperforms state-of-the-art solvers including those based on subgradient optimization and off-the-shelf linear programming solvers.

Application of the AAK theory for sparse approximation of exponential sums

V. Pototskaia (Georg-August-Universität Göttingen), G. Plonka (Georg-August-Universität Göttingen) 15:40

We derive a new method for optimal ℓ^2-approximation of discrete signals on $\mathbb{N}_0$ whose entries can be represented as an exponential sum of finite length. Our approach employs Prony's method in a first step to recover the exponential sum that is determined by the signal. In the second step we use the theory of Adamjan, Arov and Krein (AAK-theory) to derive an algorithm for computing a shorter exponential sum that approximates the original signal in the ℓ^2-norm well. AAK-theory originally determines best approximations of bounded periodic functions in Hardy-subspaces. We reformulate these ideas for our purposes and present the theory using only basic tools from linear algebra and Fourier analysis. The new algorithm is tested numerically in different examples.

S 21 : Mathematical signal and image processing

Thursday 16:30 - 18:30 Coudraystr. 13B, 2nd floor, Room 210

Shearlet-Based Morphological Component Analysis: Theory and Applications

E. King (University of Bremen), J. Murphy (Johns Hopkins University) 16:30

The basic idea behind morphological component analysis is to use collections of structurally different frames in order to perform image processing tasks like separation and inpainting via standard sparsity-based techniques. The purpose of this talk is to provide a theoretical foundation for when such an approach will be successful as well as present numerical results comparing implementations with shearlets and other systems in image processing and other types of frames in more general data processing.

The Assignment Filter: A Smooth Geometric Approach to Image Labeling

F. Savarino (Universität Heidelberg), R. Garske (Universität Heidelberg), J. Recknagel (Universität Heidelberg), F. Astroem (Universität Heidelberg), C. Schnörr (Universität Heidelberg) 16:50

The image labeling problem can be described as assigning to each pixel a single element from a finite set of predefined labels. Usually, this is done by finding optima of a globally defined objective function which evaluates the quality of a chosen labeling. Since computing global optima is in general NP-hard, various relaxations are used to yield computationally feasible problems. We propose a novel smooth geometric approach on the Riemannian manifold of stochastic matrices with full support, equipped with the Fisher Rao metric. In this setting we optimize a non-convex smooth objective function by following the Riemannian gradient flow on the manifold. This constitutes an inner approximation of the image labeling problem, implemented with interior-point numerics and parallel multiplicative updates. In addition to introducing the assignment filter, we discuss initial results relating the filter to classical discrete graphical models which, similarly to the assignment filter, maximize posterior probabilities by assigning prior features to observed data.

Shearlet frames on bounded domains

P. Petersen (TU Berlin) 17:10

Representation systems from applied harmonic analysis, such as wavelets, ridgelets, curvelets, or shearlets, have played a central role in many tasks in mathematical signal and image processing in the last couple of decades. Moreover, for instance wavelets, have been very successfully employed to discretize partial differential equations. Nonetheless, we observe a dichotomy between the theory and the applications in many of their applications since real world data, e.g., an image, is usually defined on bounded domains, whereas the systems mentioned above are mostly defined on a global domain. While for

wavelet systems there are many constructions available which also yield bases or frames on bounded domains, such a construction is mostly unknown for other systems.
In this talk we will demonstrate a quite general method to lift frame constructions from $\mathbb{R}^2$ to bounded domains by leveraging on existing wavelet frame constructions on such domains. One particular example is a shearlet frame which, with the help of our novel method, can be adapted to yield a frame on a bounded domain that admits a string of very beneficial properties. More specifically, this shearlet system is a frame for Sobolev spaces $H^s(\Omega)$ for suitable subsets Ω of $\mathbb{R}^2$. Additionally, it also admits very fast N-term approximations with respect to its primal and dual frame of functions that have curvilinear singularities. Finally, the system is efficiently computable by using well-established algorithms for the shearlet system on $\mathbb{R}^2$.
On top of that we shall demonstrate the potential of the newly developed frame for the adaptive solution of PDEs numerically. This is joint work with Massimo Fornasier, Philipp Grohs, Gitta Kutyniok, Jackie Ma, Mones Raslan, and Felix Voigtlaender.

Sparse phase retrieval of one-dimensional signals by Prony's method

R. Beinert (Karl-Franzens-Universität Graz), G. Plonka (Georg-August-Universität Göttingen) 17:30

The phase retrieval problem consists in recovering a complex-valued signal from the modulus of its Fourier transform. In other words, the phase of the signal in the frequency domain is lost. Recovery problems of this kind have many applications in physics and engineering as for example in electron microscopy, crystallography, astronomy, and communications. The long history of phase retrieval include countless approaches to find an analytic or a numerical solution, which is generally challenging due to the well-known ambiguousness of the problem.
In this talk, we consider the one-dimensional continuous-time phase retrieval problem, where we wish to recover a complex-valued signal $f\colon \mathbb{R} \to \mathbb{C}$ from its Fourier intensity $|\mathcal{F}[f]|$. In addition, we assume that the true signal f has a sparse representation of the form

$$f(t) = \sum_{j=1}^{N} c_j^{(0)}\, \delta(t - T_j) \qquad \text{or} \qquad f(t) = \sum_{j=1}^{N} c_j^{(m)}\, B_{j,m}(t),$$

where δ denotes the Delta distribution, and $B_{j,m}$ the B-spline of order m determined by the knots $T_j < T_{j+1} < \cdots < T_{j+m}$. The main question is now: can we always recover the unknown complex coefficients $c_j^{(m)}$ and the real knots T_j from the given Fourier intensity?
Using a constructive proof, we show that almost all sparse signals f consisting of N spikes at arbitrary locations can be uniquely recovered up to trivial ambiguities—up to rotations, time shifts, and conjugated reflections. An analogous result holds for the spline functions of order m. The proof itself consists of two main steps. Exploiting that the autocorrelation function A of the sparse signal f is here always an exponential sum, we firstly apply Prony's method to recover the unknown parameters (coefficients and frequencies) of A. In a second step, we use this information, which already comprise all

occurring knot differences $T_j - T_k$, to derive the unknown parameters of the signal f. On the basis of the proof, we moreover present an algorithm to recover f from $\mathcal{O}(N^2)$ intensity measurements $|\mathcal{F}[f](\omega)|$ of its Fourier transform. Finally, we illustrate the proposed method at different numerical examples.

Inflow-based finite volume method for level set equations in a polyhedron mesh

J. Hahn (AVL LIST GmbH), K. Mikula (Slovak University of Technology), P. Frolkovic (Slovak University of Technology), J. Hahn (AVL LIST GmbH) 17:50

An inflow-based gradient is proposed to solve level set equations with a cell-centered finite volume method. The proposed discretization of the magnitude of gradient is an extension of well-known Rouy-Tourin scheme; the first is that the proposed scheme can be applied in a polyhedron mesh in three dimensions and the second is that its correspondent form on a regular structured cube mesh uses the second order upwind difference. Considering a practical application in three dimensional mesh, we use the simplest decomposed domains for a parallel computation. Moreover, the implementation is very straightforward and easily combined with a conventional finite volume code. A higher order of convergence and a recovery of signed distance function from a sparse data are illustrated in numerical examples on hexahedron or polyhedron meshes.

S 22: Scientific computing

Organizers: Philipp Birken (Lund University)
Gregor Gassner

S 22 : Scientific computing

Tuesday 14:00 - 16:00 Weimar hall, Seminar room 2

Making a Common Lisp Finite Element library high-performing

N. Neuß (FAU Erlangen-Nürnberg) 14:00

We describe the optimization and parallelization of the Finite Element library Femlisp [1] using a 3D elasticity problem as a model example.
We discuss performance optimization on different levels:

1. Algorithmic improvements
2. Optimization of the serial code
3. Shared-memory parallelization

4. Distributed-memory parallelization

Since Femlisp is written in the highly dynamic language Common Lisp, we encounter several nonstandard problems before we reach a very good comprise of a code which is both dynamic and high-performing on distributed memory architectures.

1. `http://www.femlisp.org`

H-LU iteration for solving complex systems of linear equations generated by materials represented by Computed Tomography data

J. Valbuena Soler (University of Stuttgart), W. Hackbusch (Max Planck Institute for Mathematics in the Sciences), D. Uribe (University of Stuttgart), H. Steeb (University of Stuttgart) 14:40

Computing of complex effective electric permittivity and complex effective electric conductivity of porous materials plays an important role due to its applications in different fields. The numerical characterisation of materials can be carried out by studying the response of these properties under the influence of an alternating current field. The second order elliptic differential equation with varying complex coefficients has to be solved in order to compute the complex electrical properties. The continuous partial differential equation takes the following form:

$$\begin{aligned} \nabla \cdot \big[A(x,y,z)\nabla u(x,y,z)\big] &= g(x,y,z) && \text{in } \Omega \\ u(x,y,z) &= g_D && \text{on } \Gamma_D \\ \frac{\partial u(x,y,z)}{\partial n} &= g_N && \text{on } \Gamma_N \end{aligned}$$

where $A(x,y,z)$ is a second order tensor with complex coefficients that represents the electrical properties of materials. The existence of the solution of this differential equation is described in [1].

Finite Element method, Dirichlet and Neumann boundary conditions, the electrical properties of the phases in the materials are used to discretise the differential equation. The discretisation produces the system of linear equations $Lu = b$ where $L \in \mathbb{C}^{I\times I}$, and $u, b \in \mathbb{C}^I$. The special difficulties in solving the complex system are the jumping (i.e., discontinuous) coefficients due to the different phases and the complex values. This makes it complicated to find the solution of the system.

$\mathcal{H}$-LU Iteration is based on the numerical Hierarchical matrix technique that may be considered as a direct method [2]. The approach for solving the complex system of linear equations consists of using the $\mathcal{H}$-LU iteration. The performance of this scheme is measured in terms of the convergence rate. Different types of materials with their electrical properties, distinct range of frequencies, 3D tomographic images, and boundary conditions were used to build the complex systems of equations and test the scheme. The results will be discussed.

[1] J. Valbuena Soler. Solution of a Second Order Elliptic Partial Differential Equation with Varying Complex Coefficients: An Application for Computing Effective Complex Electrical Properties of Materials represented by 3D Images. PhD Thesis, Australian National University (2016). Submitted.

[2] W. Hackbusch. Iterative Solution of Large Sparse Systems of Equations. Springer International Publishing. 2nd Edition. Applied Mathematical Sciences Series (2016).

Nonlinear FETI-DP Methods for Nonlinear Problems

M. Uran (Universität zu Köln), A. Klawonn (Universität zu Köln), M. Lanser (Universität zu Köln), O. Rheinbach (Technische Universität Bergakademie Freiberg) 15:00

Parallel Newton-Krylov FETI-DP domain decomposition methods are fast and robust solvers, e.g., for nonlinear implicit problems in structural mechanics. These methods can be characterized by linearization before decomposition. By changing the order of these operations, new parallel nonlinear FETI-DP methods with increased locality and reduced communication can be designed. We introduce a unified framework, which casts all nonlinear FETI-DP domain decomposition approaches discussed in the literature into a single algorithm and describes them as different nonlinear right-preconditioners. All of these nonlinear FETI-DP methods, which are equivalent when applied to linear problems but show a different performance for nonlinear problems, will be discussed and parallel weak scaling results on up to 131K BlueGene/Q cores on JUQUEEN at FZ Jülich will be presented in this talk.

A Two-Level Overlapping Schwarz Method with GDSW Coarse Spaces for Saddle Point Problems

A. Heinlein (Mathematical Institute, University of Cologne), C. Hochmuth (Mathematical Institute, University of Cologne), A. Klawonn (Mathematical Institute, University of Cologne) 15:20

Domain decomposition methods of overlapping Schwarz type for saddle point problems, e.g., Stokes or almost incompressible elasticity are considered. We propose a scalable monolithic approach for a two-level overlapping Schwarz preconditioner. Here, the coarse space is a generalization of a known energy minimizing coarse space (GDSW) for linear second order elliptic partial differential equation. A parallel implementation for the Stokes problem based on Trilinos will be presented in the talk. Due to the fully algebraic construction of the preconditioner the use of structured grids is not necessary.

Domain-Decomposition-Based Fluid-Structure Interaction Methods Using Nonlinear Anisotropic Arterial Wall Models

A. Heinlein (Universität zu Köln), A. Klawonn (Universität zu Köln), O. Rheinbach (Technische Universität Bergakademie Freiberg) 15:40

Stress distributions in walls of in vivo arteries (transmural stresses) are a major factor

driving, e.g., arteriosclerosis and arteriogenesis. We focus on fluid-structure interaction (FSI) using sophisticated nonlinear structural models. Such models have been developed and adapted to experiments in the past. We use an anisotropic, polyconvex hyperelastic structural model. The coupled FSI problems are solved using a monolithic approach based on domain decomposition, i.e., overlapping Schwarz and Dirichlet-Neumann methods. Our solver environment combines the FEM software packages LifeV and FEAP, which provide the nonlinear models for the fluid and a nonlinear, polyconvex, anisotropic model for the structure. Furthermore, we discuss improvements in the computing time of our FSI simulations, e.g., due to the use of suitable parallel domain decomposition preconditioners.

S 22 : Scientific computing

Tuesday 16:30 - 18:30 Weimar hall, Seminar room 2

An Efficient Thermo-Kinematic (ETK) Model for Long-Time Simulation of High Speed Railway Brake Dynamics

T. Srisupattarawanit (TU Braunschweig), G. Ostermeyer, F. Schiefer 16:30

begin{document} High speed railway brakes transfer a large amount of kinetic energy into heat during the brake operation. Due to its design one majority problem is tapered wear, which could significantly reduce brake performance and safety as well as increase aftermarket costs. Modeling and Simulation of these brake systems is rather complicated with respect to the coupled multiphysics, multiscale phenomena, friction and wear, especially in long time scale. Here we present the so-called Effective Thermo-Kinematic (ETK) model, which include the complexities of the multiphysics of the brake process in the efficient way with respect to wear. Using this model, we are able to proceed the simulation of the brake dynamics in long-time scale. The partial differential equations are derived based on the coupled manner. The simulation with ETK model shows reasonable results with in very short simulation time. The ratio of computing time to real time can reach 1:2000 (with personal computer). Thus, investigations on tapered wear can be performed not only in one brake operation but in many times of brake operations. The simulation results will support the development process of railway brakes in order to mitigate tapered wear of the brake pads. \end{document}.

Distributed parallel non-equilibrium Green's function approach to inelastic charge transport

S. Achilles (Aachen Institute for Advanced Study in Computational Engineering Science (AICES)) 16:50

Inelastic charge transport is of paramount importance for simulating quantum transport in mesoscopic systems with the focus on novel nano-transistor concepts [1, 2] or quantum

photovoltaic devices [3, 4]. The widely used method for first-principle calculations of electronic structure theory computations are Density Functional Theory (DFT) methods. These DFT methods are based on the evaluation of the Kohn-Sham equations [5]. However, DFT is a ground-state theory that does not allow for the calculation of electric currents due to externally applied voltages. The Non-Equilibirum Green's Functions (NEGF) framework goes beyond this widely used DFT methods. NEGF is an advanced simulation approach that allows for the simulation of large atomic system, for treatment of transport phenomena and out-of-equilibrium transport. The NEGF formalism was simultaneously introduces by Schwinger an co-workers [6], Kadanoff and Baym [7], and Keldysh [8] and provides a quantum-statistical mechanics picture of many-body system far from equilibrium. The NEGF simulation is computationally very intense, because it includes open boundary conditions that couple the device to an out-of-equilibrium environment where electrons move due to externally applied voltages.
The computational intensity requires a massively parallel implementation to exploit the available resources of a state-of-the-art supercomputer. Four different level of parallelism are offered within the NEGF algorithm. The first level parallelism is trivial, since no dependencies are present. The next two levels are parallelized with data distribution across the nodes employing the Message Passing Interface (MPI). The last level is parallelized on the nodes level utilizing domain decomposition. Consequently the presented parallelization approach is hybrid and emphasizes the advantages of the two different worlds: distributed and shared memory paradigm.
The presented parallelization approach is scaling on up to 458,752 cores on JUQUEEN and sets the foundation for unprecedented simulations of large systems, e.g. the simulation of a complete realistic device.

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Simulating convex polyhedral particles utilizing the discrete element method

E. Siegmann (RCPE GmbH), J. Khinast (TU Graz), G. Haase (Karl-Franzens-University Graz) 17:10

Simulations of granular flows are an effective tool to gain deeper understanding of processes like fluidized beds, mixing, powder transport, etc. The discrete element method (DEM) allows simulating these kinds of processes. Each particle is treated individual and its motion is described by Newton's equation of motion. A soft-sphere approach is used, where colliding particles are allowed to slightly overlap. This overlap results in a repulsive force.

The particle shape plays an important role in order to get a realistic model of the system. There are several approaches for modelling the shapes of more complex particles. The multisphere approach clusters several spheres to one rigid body [1]. Biconvex tablets can be represented as the overlap of three spheres. Superquadrics allow modelling many shapes, such as ellipsoids, cylinder- and box-like particles [2]. To increase the accuracy particles can be modelled as convex polyhedrals [3]. This approach allows simulating sharply-edged non-spherical particles.

Where the collision of spheres is easy to handle more complex shapes are challenging. This work shows an accurate contact algorithm for arbitrary shaped convex polyhedrals. The algorithm has been implemented in the GPU based DEM software XPS, allowing to simulate a huge number of particles [4].

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2. Podlozhnyuk A., Pirker S., Kloss C. Efficient implementation of superquadric particles in Discrete Element Method within an open-source framework. Computational Particle Mechanics. 2016, S. 1-18.

3. Govender N., Wilke D.N., Kok S., Els R. Development of a convex polyhedral discrete element simulation framework for NVIDIA Kepler based GPUs. Journal of Computational and Applied Mathematics, Volume 270. November 2014, S. 386-400.

4. Jajcevic D., Siegmann E., Radeke C., Khinast J. Large-scale CFD-DEM simulations of fluidized granular systems. Chemical Engineering Science, Volume 98. 2013, S. 298-310.

A coupled ODE-PDE model for nanobubbles in hydrogen electrolysis

S. Kimmerle (Universität der Bundeswehr München) 17:30

We present a mathematical model for nanobubbles arising from the hydrogen electrolysis in polymer electrolyte membranes. Near the cathode of the electrolyser hydrogen nanobubbles emerge in protonated water. At first surface nanobubbles in the form of sperical caps are generated that may finally detach and become spherical bulk nanobubbles. These nanobubbles may grow and shrink with time. On one hand this is due to

the inflow of electrons into water at the cathode and producing hydrogen, on the other hand the surface tension enhances the dissolution of the bubbles. Experiments show that these nanobubbles have a longevity that cannot be explained by classical theory. In the context of electrolysis the generation of large meta-stable surface nanobubbles is an undesired effect.

In our model surface and bulk nanobubbles may be both parametrized by their radii. Assuming a dynamical equilibrium this yields a coupled system consisting of an advection-diffusion equation for the hydrogen concentration in water, ODEs for the radii evolution and an algebraic equation for the total conservation of hydrogen. We consider a steady-state model for a single bubble and a many bubbles model, using a mean field approach.

For the single bubble model, we consider dynamic equilibria numerically. The coupled ODE-PDE problem is solved by an fixed-point algorithm. For the many bubbles model, we derive macroscopic evolution equations by formal homogenization techniques exploiting typical scales. The resulting large dynamical systems are simulated. Here we have to pay attention to the unknown times when bubbles dissolve. Our results exhibit an interplay between surface and bulk nanobubbles similar to Ostwald ripening, where larger bubbles grow at the expense of smaller bubbles that eventually disappear. Finally, we discuss aspects of the optimal control of a simplified many bubble system.

Furthermore, we compute values for typical lifetimes of bubbles. Our results indicate that the experimentally observed meta-stability of nanobubbles may be explained by interaction effects between many nanobubbles.

The mathematical model and the single bubble problem is joint work with Knut Sverstrup (U Cambridge) and Peter Berg (U Alberta).

Computational and Experimental Determined Aerodynamic Characteristics of Flying Configurations, in Supersonic Flow (part I)

A. Nastase (RWTH-Aachen University) 17:50

Keywords: 76J20 Supersonic flow,.76N25 Flow control and optimization, 3SL70 Nonlinear second order PDE of hyperbolic type, 76D05 Navier-Stokes equations, (2010 MSC)

The exploration of supersonic flow over flying configurations (FCs) was performed by using eight models designed by the author, namely: a wedged delta wing, a double wedged delta wing, a wedged delta wing fitted with a central conical fuselage, a global optimized delta wing alone ADELA, two global optimized and fully-integrated wing-fuselage FCs FADET I and FADET II, a wedged rectangular wing and a cambered rectangular wing. The computations of lift pitching moment and of pressure coefficients on the upper side of these FCs were performed by using the own three-dimensional hyperbolic potential solutions and the own developed rapid software. The measurements of the lift, pitching moment and of the pressure coefficients on the upper side of the

models were performed in the trisonic wind tunnel of DLR Cologne, in the frame of research projects of the author, sponsored by the DFG. Correlation and interpolation software, developed by the author, were used by herself and by her young collaborators for the evaluation and for the plotting of the experimental determined lift, pitching moment and pressure coefficients on the upper side of FCs The very good agreement between the theoretical predicted lift, pitching moment and pressure coefficients of the wedged and the wedged delta wing fitted with a central conical fuselage and the measured values is here presented. For the determination of the total drag coefficients, own hybrid solutions for the Navier-Stokes layer, are proposed.

S 22 : Scientific computing

Wednesday 14:00 - 16:00 Coudraystr. 13A, 1st floor, Lecture hall 2

Space-Time Finite Element Simulation of Internal Compressible Flows

M. von Danwitz (RWTH Aachen University), M. Make, N. Hosters, M. Behr (RWTH Aachen University, Chair for Computational Analysis of Technical Systems) 14:00

In an internal combustion engine, piston rings are used to seal the combustion chamber and minimize leakage gas flow to the crank case. An equally important, yet conflicting, goal in the design of piston rings is the reduction of friction losses. In today's engines, a compromise between the two design goals leads to a measurable gas flow around the piston rings [1]. Gas flow from the combustion chamber to the crank case is denoted as blow-by; flow in the opposite direction, reverse blow-by. Our current efforts to numerically study these phenomena in two- and three-dimensional simulations are presented in this contribution.

Our solution strategy is based on the deforming-spatial-domain/stabilized space-time (DSD/SST) procedure which uses finite elements for the spatial and temporal discretization and allows computations on moving grids. The computational domain around the piston ring is composed of a large chamber with approximately 5 mm diameter and narrow channels of only 2 μm in height. To resolve the flow field in this domain as accurately as possible with a limited number of finite elements, quadrilaterals and hexahedrons with very high aspect ratio are used for the discretization.

We use an SUPG stabilization method to obtain a stable solution to the compressible Navier-Stokes equations. The definition of the required stabilization parameter includes a characteristic length scale for each element. In case of high aspect ratio elements, it is an intricate task to determine the best suitable element length scale. We will present a stabilization method with an implicit element length definition, based on [2]. The performance of this method is compared to two other stabilization methods, in which

the minimum element edge length is used as length scale [3, 4]. Finally, results of the computation of the transient compressible flow around a moving piston ring with the new stabilization method are presented.

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[4] V. Kotteda, S. Mittal. Stabilized finite-element computation of compressible flow with linear and quadratic interpolation functions. *International Journal for Numerical Methods in Fluids* 75: 273-294, 2014.

Discontinuous Galerkin schemes for space physics applications

M. Bohm (Universität zu Köln), G. Gassner 14:20

In this presentation the three-dimensional resistive MHD equations are solved by a Discontinuous Galerkin Spectral Element Method (DGSEM) on unstructured, curved meshes. Since high order approximations of nonlinear conservation laws are prone to oscillations in regions with strong shocks and contact discontinuities, special attention is paid to shock capturing strategies. More precisely, the solution is smoothed in these shocked regions by adding an appropriate amount of artificial viscosity.
Furthermore, the hyperbolic divergence cleaning for the MHD equations as well as aspects of High Performance Computing (HPC) are discussed. Finally, simulation results of a particular space physics application dealing with MHD flows through atmospheric geometries are demonstrated and compared to the state-of-the-art finite difference solver ZEUS.
Mathematics Subject Classification (2010): 65M70, 76W05

Entropy stable discontinuous Galerkin methods for the Shallow Water equations

N. Wintermeyer, G. Gassner, A. Winters (Universität zu Köln) 14:40

In this talk we describe a high-order nodal discontinuous Galerkin spectral element approximation for the two dimensional shallow water equations with non-constant, possibly discontinuous, bathymetry. The scheme operates on unstructured, possibly curved, quadrilateral meshes. The discretisation exactly preserves the local mass and momentum and fulfills an inequality for the energy, which is an entropy function for the shallow water equations. Thus, the numerical scheme discretely satisfies the second law of

thermodynamics. Finally, with a particular discretisation of the bathymetry source term we prove that the numerical approximation is well-balanced. Numerical examples verify our theoretical findings and provide an application of the scheme for a partial break of a curved dam test problem. This method has also been successfully implemented on GPUs.
Mathmatics subject classification (2010): 65M70

TU Berlin Stator Optimisation with an Adjoint CFD Method and Differentiated CAD Kernel

M. Banovic (Universität Paderborn), S. Auriemma (OpenCascade), O. Mykhaskiv (Queen Mary University of London), A. Walther (Universität Paderborn), H. Legrand (OpenCascade), J. Müller (Queen Mary University of London) 15:00

To perform a derivative-based shape optimisation of a CAD-based model, one requires the calculation of geometrical sensitivities with respect to the design parameters of the model. The accurate way of obtaining these sensitivities is to apply the Automatic Differentiation (AD) to the CAD sources. This study implemented the AD version of the open-source CAD kernel OpenCASCADE Technology using the forward mode (reverse mode integration is in progress) of AD tool ADOL-C (Automatic Differentiation by Overloading in C++). Furthermore, this differentiated CAD kernel has been coupled with a discrete adjoint CFD solver, thus having a complete design chain. To validate such a work flow, we performed a derivative-based optimisation of the total pressure loss in the TU Berlin TurboLab Stator.

A fast preconditioned additive Runge-Kutta smoother for the RANS equations

P. Birken (Lund University), J. Bull (Uppsala University), A. Jameson (Stanford University) 15:20

We consider multigrid methods for compressible turbulent flow problems. For the Reynolds averaged Navier-Stokes equations (RANS), important progress has been achieved for finite volume discretizations through a new class of preconditioned Runge-Kutta smoothers [4, 3]. Here, we consider k-step GMRES and SGS as preconditioners for additive Runge-Kutta methods [1], based on simplified discretizations.
An important part of a finite volume discretization is the flux function and it turns out that the choice of this has a strong influence on convergence of the multigrid method. We look at several variants of the Jameson-Schmidt-Turkel scheme [2]. The resulting multigrid smoothing factor is analyzed using a discrete Fourier analysis. Numerical results for steady and unsteady flows show the effectivity of the approach.

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Solving the transient incompressible Navier-Stokes problem as explicit as possible

G. Lube (Georg-August Universitaet Goettingen, NAM) 15:40

There is a renewed interest in solving the transient incompressible Navier-Stokes problem using artificial compression methods. This allows to apply explicit time- stepping methods based on CFL-restrictions on the time step and simplifies massive parallelization. On the other hand, one has to take care of non-physical acoustic waves. We report on recent attempts in this direction.

S 22 : Scientific computing

Wednesday 16:30 - 18:30 Coudraystr. 13A, 1st floor, Lecture hall 2

Accelerated Gramian Computation for Dynamical Systems on Modern Hardware

J. Saak (Max Planck Institute for Dynamics of Complex Technical Systems), M. Köhler (Max Planck Institute for Dynamics of Complex Technical Systems) 16:30

Gramian matrices play an important role in the analysis and model order reduction of linear dynamical systems in input/output formulation. They allow the easy interpretation of the energetic relevance of state components, determine certain system invariants (under state space coordinate transformations) and can also be used for the computation of important system norms. In the continuous time case the relevant Gramian matrices can, on the one hand, be expressed as matrix-valued integrals over infinite time intervals and are, on the other hand, given as solutions to Lyapunov or Sylvester matrix equations. For non-linear input/output systems, empirical Gramians extend the concept by sampling the integral expressions.
After a short introduction to the interesting Gramians, matrix equations and corresponding solvers, in this contribution, we present a BLAS level-3 type tiling approach for the solution of (generalized) Sylvester equations, including the (generalized) Lyapunov and

Stein equations, after the reduction of the coefficients to Schur form. The methods thus accelerate the triangular solution phase, compared to the existing BLAS level-2 methods, by the use of a number of efficiency improving implementation techniques. On the one hand, the proposed BLAS level-3 solvers act as an outer iteration that exploits the existing algorithms for solving the arising block problems on the single tiles. On the other hand, we optimize the existing BLAS level-2 solvers with respect to the capabilities of modern computer architectures. Beside this classical BLAS level-3/level-2 type tiling approaches, we combine the newly evolved methods with features from the latest OpenMP 4/4.5 standard to get parallel implementation, which works independent of the parallel features provided by the BLAS library.
When RECSY, the only previously existing useful BLAS level-3 solver, is used as the inner method, the outer iteration contributes a largely regularized memory access pattern. Therefore also here we get a notable acceleration with respect to the standalone solver. For a single equation the runtime is, however, dominated by the reduction of the coefficient matrices to Hessenberg/Schur form. Therefore, the overall performance gain is limited. However, the gain can be increased, e.g, when the equations with the same coefficient needs to be solve for several right hand sides. This is for example the case if autonomous differential matrix equations are solved or the condition number of the operator should be estimated.

GPU Accelerated Gauss-Jordan Elimination on the OpenPOWER platform - A case study

M. Köhler (Max Planck Institute for Dynamics of Complex Technical Systems), J. Saak (Max Planck Institute for Dynamics of Complex Technical Systems) 17:10

The solution of linear systems is still one of the basic building blocks in scientific computing. Therefore, it needs to optimized for each new hardware platform in order to satisfy the users will for a faster solution. During the last decade many of these building blocks where accelerated by the usage of GPUs and similar accelerator devices. In our contribution we will focus on the solution of linear systems with many right hand sides, where a fast solution not only requires an optimized LU decomposition. Here, we also need an efficient forward and backward substitution phase. Due to their nature the solution of linear systems with triangular matrices appearing here is a difficult task for parallelization and optimization. Therefore, we propose an all-at-once solution scheme based on the Gauss-Jordan Elimination approach, which is better parallelizable cross many GPUs than the LU decomposition with forward/backward substitution. Caused by the fact the most accelerator based algorithms are implemented as hybrid CPU-GPU code the bandwidth and the latency of the CPU – GPU interconnect is the bottleneck of the idea. Typically, this is built on top of a PCIe interconnect with a maximum speed of 16GB/s. With the newly emerged IBM OpenPOWER8+ platform this interconnect is replaced by Nvidia NVLink technology transferring the data with at least 80GB/s. This technology will pop up in the HPC landscape for example as Titan's successor Sunmit at Oak Ridge National Laboratory. We present how this architectural change influences

the runtime as well as the problem sizes that can be handled by the accelerated code. Furthermore, we check the influence on problem specific parameters like the optimal block size for the algorithm.

Fast Low-Rank Empirical Cross Gramians

C. Himpe (Max-Planck-Institut für Dynamik komplexer technischer Systeme), S. Rave (Westfälische Wilhelms Universität Münster), J. Saak (Max Planck Institute for Dynamics of Complex Technical Systems) 17:30

The cross Gramian matrix encodes the input-output coherence of linear control systems. This linear operator has applications in projection-based model reduction, which is based on the singular value decomposition (SVD) of the cross Gramian.
The empirical cross Gramian is a data-driven variant of the cross Gramian that extends to nonlinear systems. A drawback of the empirical cross Gramian for large-scale systems is its full-order and dense structure; yet, it may be computed column-wise. Using the hierarchical approximate proper orthogonal decomposition (HAPOD) instead of the SVD, this partial computability can be exploited to obtain a reducing truncated projection for model order reduction without assembling the full cross Gramian. The flexibility of the HAPOD allows a parallel or a memory economic computation depending on the compute environment and beyond the plain empirical cross Gramian further cross Gramian variants, such as the joint Gramian for combined state and parameter reduction and the non-symmetric cross Gramian can be computed by the same data-driven method.

Eigensolver methods for the Hermitian Wilson Dirac Operator in lattice QCD

A. Strebel, M. Rottmann, K. Kahl (Bergische Universität Wuppertal), A. Frommer (Bergische Universität Wuppertal (BUW)) 17:50

We present a multigrid based eigensolver for computing low-modes of the Hermitian Wilson Dirac operator, which is of particular interest in several lattice QCD applications. For the non-Hermitian case multigrid methods have already replaced conventional Krylov subspace solvers in many lattice QCD computations. Since the γ_5-preserving aggregation based interpolation used in our multigrid method is valid for both, the Hermitian and the non-Hermitian case, inversions of very ill-conditioned shifted systems with the Hermitian operator become feasible. This enables the use of multigrid within shift-and-invert type eigensolvers. We present our MPI-C implementation of a Davidson-type method, which includes several numerical improvements enabling a synergy between the outer and the inner iteration. Our method is compared against commonly used software, i.e. PARPACK and PRIMME. We show, that if all three methods are properly tuned, our method can be at least competitive to PRIMME, while both methods are noticeably faster than PARPACK.

S 22 : Scientific computing

Thursday 14:00 - 16:00 Coudraystr. 13A, 1st floor, Lecture hall 2

Project scheduling under uncertainty and resource constraints

V. Hartmann (Bauhaus-Universität Weimar), T. Lahmer (Bauhaus-Universität Weimar), K. Smarsly (Bauhaus-Universität Weimar) 14:00

Construction project schedules provide information on the tasks to be executed, comprising durations, relations, and resource constraints. In the 1950s, the so-called critical path method (CPM) has been developed for scheduling projects. According to CPM, technical constraints are translated into precedence relations between the respective tasks and a network plan is developed accordingly. Based on given durations for each task, start and end dates of the task can now be determined. The end date of the task that finishes last equals the makespan of the entire project. Although CPM does not take into account resource constraints and uncertainties in the input data, which is a significant disadvantage, CPM is still widely used in project scheduling. Not considering resource constraints when creating a schedule results in problems during the realization phase. Tasks may not be started at the scheduled date because of resources not being available until a later point in time. Scheduling tasks accounting for their precedence relations by assuring a feasible resource distribution is a complex combinatorial problem. While exact procedures for creating schedules that account for technical and resource constraints exist, the applicability of such procedures to solve real-scale problems is limited, due to the computational effort. To this end, heuristic algorithms as well as metaheuristic algorithms have been proposed for such scheduling. While creating a first version of a project schedule, many boundary conditions are not fully known; the schedule is, therefore, based on uncertain data. The reasons for the input data being uncertain are manifold, but the consequences of such uncertainties can usually be expressed through prolonged process durations. The definition of stochastic variables as process durations instead of discrete values is therefore an appropriate way of taking uncertainties into account. One of the first approaches dealing with uncertain process durations is the program review and evaluation technique (PERT). However, PERT contains systematic errors; hence, results of this technique are unreliable. Monte Carlo simulation as a means of determining the makespan of a project with process durations defined by stochastic variables, as used in this paper, has proven to be a useful alternative. This paper emphasizes the focus on construction project schedules in civil engineering. The approach proposed in this paper takes resource constraints as well as uncertain process durations into account. The purpose of using variable process durations is not to describe start and end dates as well as the makespan by stochastic distributions, as this is of little merit in the construction world. Rather, the results obtained by the Monte Carlo simulation are used to quantify the ability of the schedule to absorb deviations from the initial schedule during the realization phase. Alternative schedules are generated by

varying the resource allocation as well as by considering alternative processes reflecting alternative construction methods for realizing the same task. These alternative schedules are then compared with respect to their ability of absorbing deviations, which enables optimizing a schedule not only with respect to a minimum makespan, but to a maximum robustness.

Real-time model adaptation

S. Chen (Universität Bremen), C. Büskens (Universität Bremen) 14:20

Solving an engineering problem starts with the description of the problem in mathematical formulas and the identification of parameters. The generated model is then used to simulate the behavior of the underlying system. However, most systems are not static. They change over time. Thus, the model needs to be adapted to these activities otherwise the predictions are wrong.
A data driven modeling method has been developed. The resulting models are adaptable in real time which is necessary for an application during operation. The approach is tested on the real application of a gas engine. This engine has been renovated to improve the performance. The differences in the power production are significant, so that the old model cannot be used anymore. The development of a new model costs a lot of time, especially if a physics based modeling method is used. Therefore, the fastest and easiest way is to adapt or update the model.
Different models are created for this example. At first the old model is checked against the measured data after the renovation to demonstrate the problem. Next, model updates are generated with different forgetting rates and they are compared to each other and to a new model which is created by the underlying data driven approach of the update. Using this comparison a recommendation is given which method is to be favored and what needs to be considered if an adaptation is applied.

HAPOD - Fast and Simple Distributed POD Computation

C. Himpe (Max-Planck-Institut für Dynamik komplexer technischer Systeme), T. Leibner (WWU Münster), S. Rave (WWU Münster) 14:40

Proper Orthogonal Decomposition (POD), or Principal Component Analysis (PCA), is a widely used technique for the construction of low-dimensional approximation spaces from high-dimensional input data. For large-scale applications and an increasing amount of input data vectors, however, computing the POD often becomes prohibitively expensive. In this contribution we introduce a generic, easy to implement approach to compute an approximate POD based on arbitrary tree hierarchies of worker nodes, where each worker computes a POD of only a small amount of input vectors. The tree hierarchy can be freely adapted to optimally suit the available computational resources. In particular, this hierarchical approximate POD (HAPOD) allows for both, simple parallelization with low communication overhead, as well as live sequential POD computation under restricted memory capacities. We will present rigorous error estimates and numerical examples which underline the performance and reliability of our approach.

[1] C. Himpe, T. Leibner, S. Rave, *Hierarchical Approximate Proper Orthogonal Decomposition*, arXiv: 1607.05210 (2016).

Crack Detection in Experimental Data by Means of a Spiking Response Model

F. Leichsenring (Institut für Statik und Dynamik der Tragwerke, TU Dresden), W. Graf (Institut für Statik und Dynamik der Tragwerke, TU Dresden), M. Kaliske (Institut für Statik und Dynamik der Tragwerke, TU Dresden) 15:00

In engineering tasks, multiple types of neural networks, such as e.g. feed-forward neural networks (FNN) or radial basis function neural networks (RBFN) are common solution methods for a wide scope of appilcations [1, 2]. Beside the different kinds of artificial neural networks, spiking neural networks (SNN) represents a continuous development in information processing within the computational units of a net.

In the contribution, the Spiking Response Model (SRM) [3], a derivative of the Hodgkin-Huxley model is utilized, whereas the specific properties of this neural type are used in order to facilitate the evaluation of uniaxial tension test data sets of carbon reinforced concrete specimens. The evaluation procedure of the experimental data targets the identification of major crack appearance based on the load cell data. For reasons of comparison and standardization, numerous uniaxial experiments are performed within the large-scale research project Carbon Concrete Composite C^3. Crack detection is considered as showcase for further development of evaluation methods based on SNNs with focal point to engineering experiments.

Essential for the evaluation is the transition of the experimental data (load cell data) to the neural temporal domain. Therefore, rate coding [5] is applied resulting in a presynaptic spike train. The actual detection of cracks in the presynaptic spike train is carried out by an evaluation neuron. The heuristic approach is validated by multiple examples and presents a sufficient accuracy as well as it retains the temporal information regarding the crack occurrence. A feed-forward network structure containing additional evaluation neurons in combination with extra experimental data (e.g. strain gauges) enables extended information extraction such as determining crack location with respect to the attached strain gauges.

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Numerical Shape Optimization to Decrease Failure Probability of Ceramic Structures

C. Hahn (Universität Kassel), M. Bolten (Universität Kassel), H. Gottschalk (Bergische Universität Wuppertal) 15:20

Ceramic is a material frequently used in industry because of its favorable properties. Due to its popularity shape optimization is needed in these industrial applications. Common approaches in shape optimization for ceramic structures concerning tensile loading aim to minimize the stress acting on the component, as it is the main indicator for failure. In contrast to this we follow a more natural approach by minimizing the component's probability of failure. For this purpose and in full consideration of fracture mechanics matters, the objective functional describing this probability of failure for a given ceramic component under one tensile load was recently established. With this objective functional the problem is stated as a PDE constrained optimization problem. To solve the minimization problem, we choose a gradient based method combined with a first discretize then optimize approach. For discretization finite elements are used. By converting the objective functional with the help of the Lagrange function we are able to calculate the shape gradient. The implementation was verified by comparison of it with a finite difference method applied to a minimal 2d example. This demonstrated that the calculated shape gradient actually points towards the direction of the optimal shape in terms of the failure probability. In this talk we present the objective functional as well as our implementation and some numerical examples.

The Z-matrix algorithm for the validation of measured data in process plants

E. Zander (Technische Universität Braunschweig) 15:40

The stationary state of a process or power plant is usually governed by a set of balance and rate equations. Measuring a subset of the state variables allows to estimate some of the unmeasured quantities, but may also lead to contradictory results in some of the balance equations. Using the uncertainty in the measurements, usually given by confidence intervals, an equilibrated state fulfilling the balance equations, equivalent to a MAP estimate, plus the remaining uncertainty in this state estimate may be computed. In Germany this process is described by the VDI-Richtlinie 2048 for power plants. This guideline is, however, unsuitable for usage in an automated process simulation program, as it requires manual elimination of unmeasured variables. The Z-matrix algorithm described in this talk allows for efficient computation of the equilibrated state without any elimination step and of the posterior uncertainty in this state estimate.

S 22 : Scientific computing

Thursday 16:30 - 18:30 Coudraystr. 13A, 1st floor, Lecture hall 2

Goal Oriented Time Adaptivity using Local Error Estimates

P. Meisrimel (Lund University), P. Birken (Lund University) 16:30

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When solving ODEs or PDEs, one is not always interested in the solution $\mathbf{u}(t)$, but rather a functional of the solution. Starting from an ODE (semidiscretized PDE), we consider functionals of the form

$$J(\mathbf{u}) = \int_{t_0}^{t_e} j(\mathbf{u}(t))dt$$

with $j : \mathbb{R}^n \to \mathbb{R}$. Examples for this are determining the net-flow of mass in an engine, the average energy production of a turbine or the drag coefficient for a vehicle.
The standard approach for controlling the error in the quantity of interest $J(\mathbf{u})$ is the method of weighted residuals [1], which is used to estimate the error in the quantity of interest. This method requires solving the given ODE (PDE) forward in time and its adjoint problem backwards in time multiple times each, to reach a desired precision.
An alternative approach is to use time-adaptive schemes based on local error estimates [2], which require only one forward solve, at the cost of losing the error estimate in $J(\mathbf{u})$.
We propose a new method to get the best of both worlds, we aim to reach a desired precision in a single forward solve. We take the local error approach, but determine the timesteps using only the quantities that are relevant for $J(\mathbf{u})$.
In the talk, an analysis of this method and numerical results of the new method will be presented.

[1] Becker, Roland and Rannacher, Rolf An optimal control approach to a posteriori error estimation in finite element methods
Acta Numerica 2001, Volume 10, pages 1–102, Cambridge Univ Press

[2] Shampine, Lawrence F Numerical solution of ordinary differential equations
Volume 4, 1994, CRC Press

Multirate finitesimal step methods with varying stepsizes

A. Naumann (TU Dresden), J. Wensch (TU Dresden) 16:50

Many partial differential equations consist of slow and fast scales. Often, the right hand side of semidiscretized PDEs can be split additively in corresponding fast and slow parts.

Many methods utilise the additive splitting of these equations, like generalized additive Runge-Kutta (GARK) methods or multirate infinitesimal step methods. The latter one treat the slow part with macro step sizes, whereas the fast part is integrated with small steps of an auxiliary ODE. The corresponding order conditions assume the exact solution of the auxiliary ODE, i.e. assume an infinite number of small steps. We extend the MIS approach by fixing the number of steps, which leads to the multirate finitesimal steps (MFS) method. The order conditions will be derived, such that the order is independent in the number of small steps in each stage. Finally, we confirm the theoretical results by numerical experiments.

Asymptotic Stability of Autonomous (P)DAEs with Network Structure

C. Tischendorf (Humboldt-Universität zu Berlin) 17:10

We analyze autonomous differential algebraic equations (DAEs) with the following particular structure:

$$\begin{aligned} y_1' &= \frac{\mathrm{d}}{\mathrm{d}t} f_1(x_1) + g_1(x_1), \\ x_2' &= \frac{\mathrm{d}}{\mathrm{d}t} f_2(y_2) + g_2(y_2), \\ x_1 &= A_1^\top z, \\ x_2 &= A_2^\top z, \\ 0 &= A_1 y_1 + A_2 y_2, \end{aligned}$$

where (A_1, A_2) is an incidence matrix of full row rank. First we show that a transient modeling of the flow of different kind of networks (circuits, water networks, gas networks, blood circuits) leads to DAEs with this structure. The functions f_1, f_2, g_1, g_2 represent the element models and their spatial discretizations (in case of PDE element models). The matrices A_1, A_2 describe the network topology. Furthermore we show the equivalence to a Port-Hamiltonian system in the special case that A_1 is nonsingular and f_1, g_1 are globally invertible.
Finally we present criteria on the element model functions f_1, f_2, g_1, g_2 for asymptotic stability of DAEs with this structure. It includes a characterization of the eigenvalue structure for the related generalized eigenvalue problem of the form

$$\begin{aligned} y_1 &= \lambda F_1 x_1 + G_1 x_1, \\ x_2 &= \lambda F_2 y_2 + G_2 y_2, \\ x_1 &= A_1^\top z, \\ x_2 &= A_2^\top z, \\ 0 &= A_1 y_1 + A_2 y_2. \end{aligned}$$

A Convergence Criterion for the Gauss-Seidel Waveform Relaxation Applied to Index-2 Circuit DAEs

J. Pade (HU Berlin), C. Tischendorf (HU berlin) 17:30

While waveform relaxation methods converge for coupled ODE systems, they may suffer from instabilities for coupled differential-algebraic equations (DAEs). Several convergence criteria are known for index-1 DAEs. We present here a convergence criterion for quasilinear index-2 DAEs for the first time. It applies to systems of spatially discretized Maxwell equations for electromagnetic field approximation included into lumped circuit equations for transient simulation. Such systems appear in co-simulation approaches for coupled EM/circuit simulation. The circuit topology can be exploited and makes it relatively easy to check if the convergence criterion is satisfied.

Multiharmonic analysis for nonlinear acoustics with small excitation amplitude

A. Thöns-Zueva (TU Berlin) 17:50

Acoustic experiments show that the noise absorption by perforated walls differs if small or large acoustic amplitudes are used. In addition, an interaction between different frequencies has been observed. To describe these effects we consider the compressible Navier-Stokes equations in time domain with the nonlinear advection term, which couples velocity and pressure. Here, we consider small amplitudes of the excitation and viscosities like $O(\varepsilon^2)$ with some small parameter ε. Nonlinear acoustics can be described in frequency domain by the multiharmonic analysis applied to the compressible Navier-Stokes equations, which takes into account the frequency ω of the incoming wave and their harmonics $0\omega, 2\omega, 3\omega, \ldots$. With an asymptotic expansion for small viscosities and amplitudes, both scaled like ε^2, we obtained corrector terms of order 1 and 2 for frequency 0, ω, and 2ω, where the static contribution of order 1 couples with the second order solution for $k = 1$.
Based on joint work with K. Schmidt.

S 23: Applied operator theory

Organizers: Rainer Picard
Sascha Trostorff (TU Dresden)

S 23 : Applied operator theory

Tuesday 14:00 - 16:00 Weimar hall, Seminar room 3

New spectral bounds for damped systems

C. Tretter (University of Bern), B. Jacob (Bergische Universität Wuppertal), C. Trunk, H. Vogt (Universität Bremen) 14:00

In this talk new enclosures for the spectrum of non-selfadjoint operator matrices associated with second order linear differential equations $\ddot{z}(t) + D\dot{z}(t) + A_0 z(t) = 0$ in a Hilbert space will be presented. These new bounds are obtained by means of the so-called quadratic numerical range and improve classical numerical range bounds considerably. An application to small transverse oscillations of a horizontal pipe carrying a steady-state flow of an ideal incompressible fluid illustrates that our new bounds are explicit.

Input to state stability of evolution equations

B. Jacob (Bergische Universität Wuppertal), R. Nabiullin, J. Partington, F. Schwenninger (Universität Hamburg) 14:20

In this talk we will study the notion of input to state stability for boundary control systems, which is a stronger notion then exponential stability of the corresponding semigroup and includes stability with respect to input functions as well. It will be shown that in particular parabolic boundary control systems are input to state stable. Moreover, related notions like integral input to state stability are studied and sufficient conditions are derived.

Functional calculus and admissibility

F. Schwenninger (Universität Hamburg), B. Jacob (Bergische Universität Wuppertal), H. Zwart 14:40

We will present recent progress in the study of L^∞-admissibility. This is in line with recent developments in the study of input-to-state stability for infinite-dimensional systems. We show how these notions can be linked to the boundedness of the H^∞ calculus.

Dichotomy properties of unbounded linear operators

C. Wyss (Bergische Universität Wuppertal) 15:00

A linear operator S on a Banach space V is called dichotomous if the imaginary axis is contained in the resolvent set of S, and there is a direct sum decomposition $V = V_+ \oplus V_-$ into invariant subspaces corresponding to the spectrum in the right and left half-plane.

In this talk we present various results ensuring first the existence of a spectral gap along the imaginary axis and then the dichotomy of S. In some cases however, although the invariant subspaces $V_\pm$ exist, their sum $V_+ \oplus V_-$ will only be dense in V. The results make use of different structures of S, e.g. bisectoriality or a block operator matrix structure of some kind.

S 23 : Applied operator theory

Tuesday 16:30 - 18:30 Weimar hall, Seminar room 3

Abstract boundary delay systems and application to flow in network with memory

A. Bátkai (PH Vorarlberg) 16:30

In many cases partial differential equations can be modelled as abstract boundary value problems. Based on the theory of infinite dimensional regular systems we study a class of boundary perturbation problems with distributed and boundary delay terms.
As an application we consider a flow in a network with unbounded delays. We prove well-posedness and present conditions on asymptotic stability of such equations.
Joint work with S. Hadd, M. Kramar Fijavž and A. Rhandi.
A. Bátkai, M. Kramar Fijavž, and A. Rhandi, *Positive Operator Semigroups: from Finite to Infinite Dimensions*, Operator Theory: Advances and Applications 257,Birkhäuser-Verlag, Basel, 2017.

A canonical decomposition for linear relations

H. Winkler (TU Ilmenau/ Fak. MN), T. Berger (Institut für Statik und Dynamik der Tragwerke, TU Dresden), H. de Snoo, C. Trunk 16:50

The structure of a linear relation (multivalued operator) in a finite-dimensional space is completely determined. Three different types of linear relations in finite-dimensional spaces are presented:

1. *Multishifts*, i.e., injective relations without eigenvalues;
2. *Jordan relations*, i.e., relations with a finite number of eigenvalues (including possibly ∞), which are made up of the corresponding Jordan chains;
3. *Completely singular relations*, i.e., multivalued relations which are made up of so-called singular chains; their eigenvalues fill up the set of complex numbers including ∞.

It is shown, that any linear relation can be written as a reduced sum of a Jordan relation, a completely singular relation, and a multishift.

Numerical range with respect to a family of projections

W. Dada (University of Wuppertal) 17:10

I will introduce in this talk the concept of the numerical range of a bounded linear operator with respect to a family of projections and give a precise definition and elaborate on its connection to the classical numerical range as well as to generalisations such as the quadratic numerical range and block numerical range. Most importantly, the introduced notion of numerical range illustrates that the classical numerical range can be obtained completely from spectral properties of the operator. This work is the joint work with N. Erkurşun and J. Kerner.

Eigenvalues of rank one perturbations of Hermitian matrix pencils

H. Gernandt (TU Ilmenau) 17:30

We consider regular Hermitian matrix pencils and describe the behavior of the eigenvalues under Hermitian rank one perturbations. For a given matrix pencil, we characterize which sets in the complex plane arise from Hermitian rank one perturbations. Special attention is paid to the perturbation of definite type spectrum of J-Hermitian matrices.

Eigenvalue estimates for singular indefinite Sturm-Liouvillle differential operators

P. Schmitz (TU Ilmenau) 17:50

In this talk Sturm-Liouville differential operators related to the singular differential expression

$$\frac{1}{r}\Big(-\frac{\mathrm{d}}{\mathrm{d}x}p\frac{\mathrm{d}}{\mathrm{d}x}+q\Big)$$

on the real line are considered. Here the weigh r is an indefinite function. Explicit bounds on non-real eigenvalues under certain conditions on the coefficients r, p and q are introduced. These bounds are basically linked to the L^1-norm of the potential function q. This talk is based on a joint work with Jussi Behrndt (TU Graz) und Carsten Trunk (TU Ilmenau).

S 23 : Applied operator theory

Wednesday 14:00 - 16:00 Coudraystr. 11C, Room 101

L_∞-estimates for the torsion function and L_∞-growth of semigroups satisfying Gaussian bounds

H. Vogt (Universität Bremen) 14:00

The torsion function u_D of an open set $D \subseteq \mathbb{R}^d$ can be defined as follows: $u_D(x)$ is the expected time for the Brownian motion starting at x to leave the set D. Let Δ_D

denote the Dirichlet Laplacian acting in $L_2(D)$, with ground state energy $E_0(-\Delta_D) := \inf\sigma(-\Delta_D)$. If $E_0(-\Delta_D) > 0$, then the torsion function u_D is the unique solution of $-\Delta_D u = 1$.
We show that

$$1 \le E_0(-\Delta_D) \cdot \|u_D\|_\infty \le \frac{d}{8} + 0.61\sqrt{d} + 1. \tag{1}$$

The constant in the right hand side is quite sharp: If B_d is the unit ball in $\mathbb{R}^d$, then

$$\frac{d}{8} \le E_0(-\Delta_{B_d}) \cdot \|u_{B_d}\|_\infty \le \frac{d}{8} + Cd^{1/3}$$

with some absolute constant $C > 0$. The second inequality in (1) is derived from a suitable L_∞-estimate for the semigroup generated by Δ_D.

Limit operator techniques for operators on groups

C. Seifert (TU Hamburg-Harburg), R. Hagger, M. Lindner 14:20

We consider bounded operators on $L_p(G, \mu)$-spaces, where G is a group with Haar measure μ and $p \in (1, \infty)$. By using limit operator techniques we provide a description of the essential spectrum in terms of the spectra of the corresponding limit operators in a general framework.

A Limit-Point- and Limit-Circle Classfification of second-order differential operators and their application to PT -symmetric quantum mechanics

F. Leben (TU Ilmenau), C. Trunk 14:40

We consider a second-order differential equation $-y'' + q(x)y(x) = \lambda y(x)$ with complex-valued potential q and eigenvalue parameter λ. In $\mathcal{PT}$-symmetric quantum mechanics x is on a contour $\Gamma \subset \mathbb{C}$. If the contour Γ is chosen in a very simple way, $\Gamma := \left\{xe^{i\phi \mathrm{sgn} x} : x \in \mathbb{R}\right\}$, then the above problem splits into two differential equations on the semi-axis $[0, \infty)$ and on $(-\infty, 0]$, respectively. We provide a limit-point-limit-circle-classification of this problem with the help of asymptotic analysis (WKB). Moreover we obtain enclosures for the spectrum of the operators.

Explicit solutions of dynamical canonical, Dirac-Weyl and Schrödinger systems

A. Sakhnovich (University of Vienna) 15:00

We discuss interesting connections between so called "spectral" systems and dynamical systems (i.e., systems with additional dependence on time). In particular, using our GBDT version of Bäcklund-Darboux transformation we construct and analise explicit solutions of important dynamical systems [1,2]. Using procedures of solving inverse problem for the spectral Dirac system, one can recover dynamical Dirac system from the response function [3].

[1] A.L. Sakhnovich, Dynamical canonical systems and their explicit solutions,

arXiv:1603.08709v2, Discrete and Continuous Dynamical Systems Series A to appear.

[2] A.L. Sakhnovich, Dynamics of electrons and explicit solutions of Dirac-Weyl systems, arXiv:1609.03451.

[3] A.L. Sakhnovich, Dynamical and spectral Dirac systems: response function and inverse problems, J. Math. Phys. 56 (2015), 112702, 13 pp.

ANTIPLANE STRAIN (SHEAR) OF NON-HOMOGENEOUS PRISMATIC SHELL-LIKE BODIES

N. Chinchaladze (Iv. Javakhishvili Tbilisi State University (TSU)) 15:20

Antiplane strain (shear) of an orthotropic non-homogeneous prismatic shell-like body is con- sidered when the shear modulus depending on the body projection (i.e., on a domain lying in the plane of interest) variables may vanish either on a part or on the entire boundary of the projection ([1,2]). The dependence of well-posedeness of boundary conditions on the character of vanishing the shear modulus is studied. Vibration problem is considered. The classical and weak setting of the boundary value problems are considered. Appropriate weighted functional spaces are introduced. Uniqueness and existence results for the variational problem are proved. The structure of the constructed weighted space is described and its connection with weighted Sobolev spaces is established.

[1] G. Jaiani (2015). Antiplane strain (shear) of isotropic non-homogeneous prismatic shell-like bod- ies, Bull. TICMI, 19, 2, 40-54.
[2] N. Chinchaladze (2015). On some dynamical problems of the antiplane strain (shear) of isotropic non-homogeneous prismatic shell-like bodies, Bull. TICMI, 19, 2, 55-65.

S 23 : Applied operator theory

Wednesday 16:30 - 18:30 Coudraystr. 11C, Room 101

On Grad - grad, div - Div, and Rot - Rot^t complexes for problems related to the biharmonic equation and elasticity.

D. Pauly (UDE) 16:30

We show that certain $Grad-grad$, $div-Div$, and $Rot-Rot^t$ complexes for problems related to the biharmonic equation and elasticity are closed and even exact for bounded and topologically trivial domains. Moreover, we prove corresponding compact embeddings, Friedrichs/Poincare type inequalities, and Helmholtz and regular type decompositions. Hence the involved solution operators are continuous and even compact. Applications for biharmonic equations and elasticity will be indicated.

Resolvent estimates in the homogenisation of one-dimensional viscoelasticity

M. Waurick (University of Bath), S. Cooper (University of Bath), K. Cherednichenko (University of Bath) 16:50

In the talk we discuss the asymptotics of the resolvents of fractional-elasticity pointwise in the frequency domain. The coefficients are periodic and as a technical tool one employs the Gelfand transform as well as a suitable decomposition of the underlying spatial Hilbert space.

Coherent structure detection by spectral analysis of a dynamic Laplace-Beltrami operator

D. Karrasch (TU München), J. Keller (TU München) 17:10

We define Lagrangian coherent structures as maximal material subsets whose advective evolution is maximally persistent to weak diffusion. For their detection, we transform flow information from advection–diffusion dynamics into a deformed Riemannian geometry on the set of initial conditions/material points. Then, Lagrangian coherent structures express themselves as those subsets of the material manifold which are particularly slowly decaying under the heat flow induced by the geometry, i.e., as metastable or almost-invariant sets under the geometric heat flow. These can be detected by a spectral analysis of the generating Laplace-Beltrami operator. We will demonstrate our method on a simple example.

Approximation of the mean-field polaron dynamics in the weak-coupling limit

J. Schmid (University of Stuttgart) 17:30

We consider the dynamics of the mean-field polaron in the weak-coupling limit of vanishing electron-phonon interaction, $\varepsilon \to 0$. This is a singular limit formally leading to a Schrödinger–Poisson system that is equivalent to the nonlinear Choquard equation. By establishing estimates between the approximation obtained via the Choquard equation and true solutions of the original system we show that the Choquard equation makes correct predictions about the dynamics of the polaron mean-field model for small values of $\varepsilon > 0$. Joint work with M. Griesemer and G. Schneider (arXiv:1609.00954).

A note on causal and amnesic operators

S. Trostorff (TU Dresden) 17:50

We provide a representation for causal and amnesic translation-invariant linear operators in terms of operator-valued functions of the derivative, established as a normal operator on a suitable Hilbert space. The results allow for a characterisation of those evolutionary equations, which do not show memory effects.

Index of persons