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Abstracts

Uniting auxeticity with extreme strength and high stiffness - the microstructure of limpet teeth

Swantje Bargmann

University of Wuppertal, Chair of Solid Mechanics, Gaußstr. 20, 42119 Wuppertal, Germany

Abstract Materials exhibiting a negative Poisson's ratio, which is also known as auxeticity, have been identified in both natural and engineered contexts, achieved through a variety of structural mechanisms. However, these typically adopt designs with lower stiffness due to the necessity of accommodating structural unit rotation or folding within available space. Consequently, the challenge of integrating auxeticity with high strength and stiffness has persisted. Our work explores the mechanical properties of limpet teeth, a material that performs remarkably well under demanding loading conditions. By employing in-situ nanomechanical testing within SEM and TEM, coupled with detailed investigations of its high-resolution structure and microstructure-based modeling, we unveil how the leading part of limpet teeth successfully attains this exceptional blend of properties.

Joint work with SH. Oh, J.-K. Kim, Y. Liu, M. Wurmshuber, X.-L. Peng, J. Seo, J. Jeong, Z. Wang, J. Wilmers, C. Soyarslan, J. Kim, B. Kittiwirayanon, J. Jeong, H.-J. Kim, Y. H. Huh, D. Kiener, H. Gao.

Wurmshuber, J. Wilmers, J. Kim, S.H. Oh, S. Bargmann, D. Kiener Lower hardness than strength: the auxetic composite microstructure of limpet tooth, Acta Biomaterialia 166, 447-453, 2023

SH. Oh, J.-K. Kim, Y. Liu, M. Wurmshuber, X.-L. Peng, J. Seo, J. Jeong, Z. Wang, J. Wilmers, C. Soyarslan, J. Kim, B. Kittiwirayanon, J. Jeong, H.-J. Kim, Y. H. Huh, D. Kiener, S. Bargmann, H. Gao Limpet teeth microstructure unites auxeticity with extreme strength and high stiffness, Science Advances 8 (48), eadd4644, 2022

Bargmann, B. Klusemann, J. Markmann, J. Schnabel, K. Schneider, C. Soyarslan, J. Wilmers Generation of 3d representative volume elements for heterogeneous materials: a review Progress in Materials Science 96, 322-384, 2018

Regularity problems for anisotropic models

Kateryna Buryachenko

HU Berlin, Angewandte Analysis, Unter den Linden 6, 10099 Berlin, Germany

Abstract The talk is devoted to the study of qualitative properties (potential estimates, asymptotic behavior, boundedness, solution regularity) for elliptic and parabolic anisotropic equations (as well as their variational interpretation) of diffusion-absorption structure with non-standard growth conditions and external sources as well as related variational problems.

Quantitative stochastic homogenization of variational models arising in fracture mechanics

Nicolas Clozeau

ISTA, Am Campus 1, 3400 Klosterneuburg, Austria

Abstract I will present a recent quantitative result concerning the homogenization of the so-called Griffith type model arising in fracture mechanics. Since the work of Cagnetti, Dal Maso, Scardia and Zeppieri, the homogenized model has been identified qualitatively and in particular the two main constitutive properties of the system have been derived : the homogenized elastic energy and the homogenized fracture toughness, both given explicitly by means of cell-formulas. I will explain in this talk how we can derive quantitative estimates for the convergence of the cell-formula for the effective toughness. This is based on a joint work with Julian Fischer and Antonio Agresti.

A variational perspective on auxetic metamaterials of checkerboard type

Dominik Engl

KU Eichstätt-Ingolstadt, Lehrstuhl für Analysis, Ostenstraße 28, 85072 Eichstätt, Germany

Abstract Auxetic metamaterials are specifically designed to have the counter-intuitive property of a negative Poisson's ratio, meaning they expand perpendicular to applied forces under stretching. In this talk, we discuss homogenization via Gamma-convergence for elastic materials with stiff checkerboard-type heterogeneities under the assumption of non-self-interpenetration. Our result rigorously confirms these structures as auxetic. The challenging part of the proof is determining the admissible macroscopic deformation behavior, or in other words, characterizing the weak Sobolev limits of deformation maps whose gradients are locally close to rotations on the stiff components. To this end, we establish an asymptotic rigidity result showing that, under suitable scaling assumptions, the attainable macroscopic deformations are affine conformal contractions. Our strategy is to tackle first an idealized model with full rigidity on the stiff tiles and then transfer the findings to the model with diverging elastic constants. The latter requires a new quantitative geometric rigidity estimate for non-connected touching squares and a tailored Poincaré-type inequality for checkerboard structures. This is joint work with Wolf-Patrick Düll (University of Stuttgart) and Carolin Kreisbeck (KU Eichstätt-Ingolstadt).

Microcharges and Microbubbles and their impact on Macroscopic behavior

Gilles Francfort

New York City University, Flatiron Institute, 162 5th Ave, New York, NY 10010, USA

Abstract I will actually focus exclusively on fluid micro-bubbles in an elastomer. I will show that elastic enhancement can be promoted through surface tension in spite of the presence of fluid filled cavities that should a priori contribute to the inverse phenomenon, namely a weakening of the material, at least in shear.

This is joint work with J. Casado Díaz (Sevilla), O. Lopez-Pamies (Urbana Champaign) and M.G. Mora (Pavia).

Variational formulation of coupled chemo-mechanics in elastic and dissipative solids

Swaroop Gaddikere Nagaraja

Montanuniversität Leoben, Lehrstuhl für Mechanik, Franz-Josef-Straße 18, A-8700 Leoben, Austria

Abstract A variational formulation for coupled chemo-mechanical problems in elastic and dissipative solids at infinitesimal strains is outlined in the present work. In doing so, it is seen that the gradient of the primary fields additionally enter the energetic and dissipative potential functions, resulting in additional balance equations. The governing balance equations of the coupled problem are derived as Euler equations of the incremental variational principles, formulated in continuous-and discrete-time settings. Furthermore, the variables governing the inelastic process are locally condensed which yields a reduced global problem that is solved in a discrete-space-time setting. The symmetric structure of the proposed framework with respect to the primary and state variables is an advantage, and this is exploited in the numerical treatment within the finite element paradigm. The framework is applied to Cahn-Hilliard- type diffusion and Allen-Cahn-type phase transformation in elastic and dissipative solids. The applicability of the proposed framework is demonstrated by means of two- and three-dimensional representative numerical simulations.

An Analysis of a Class of Variational Models for Heterogeneous Phase Separation

Likhit Ganedi

RWTH Aachen University, Lehrstuhl für Mathematik (Analysis), Templergraben 55, 52062 Aachen, Germany

Abstract We study phase separation of heterogenous mixtures of fluids. We will survey physical motivation and recent works, where variants of the famous Modica-Mortola functional are used to model this phenomenon. The specific homogenized energy of the system will depend on the relative size of the scale of the heterogeneities and phase separation. We will specifically discuss recent results in some of the regimes which also extend to the case of thermally responsive fluid phases. This is based on joint work with Riccardo Cristoferi (Radboud University) and Irene Fonseca (Carnegie Mellon University).

An Anisotropic Poincare Inequality in $GSBV^p$ and an Application to an Anisotropic Mumford-Shah Energy

Janusz Ginster

HU Berlin, Angewandte Analysis, Unter den Linden 6, 10099 Berlin, Germany

Abstract In this talk we discuss a Poincare inequality for functions in $GSBV^p$ that have a small variation in 2 of 3 spatial directions. It will be shown that such a function is close to a function of one variable outside an exceptional set. For the exceptional set bounds on the volume and the perimeter in two directions are provided. As a key tool we prove an approximation result for such functions. For this we present a two-dimensional countable ball construction that allows to carefully remove the jumps of the function. As a simple application, we present the Gamma-convergence of an anisotropic three-dimensional Mumford-Shah model to a one-dimensional model.

Multiscale Homogenisation of Diffusion in enzymatically-calcified hydrogels

Marc Graham

TU Berlin, Strukturmechanik und Strukturberechnung, Straße des 17. Juni 135, 10623 Berlin, Germany

Abstract Hydrogels are being used in an ever-widening range of applications. Although there is a large variety of hydrogel types, one common feature of them has been their lack mechanical strength, which presents a considerable limitation to their application. By adding a secondary microstructure to the material, enzymatic calcification addresses this and can produce materials capable of withstanding high loads, such as when they serve as a pressure boundary in filtration, or as a tissue scaffold in vitro or in vivo.

In such cases diffusion plays a critical role to the use case, especially where biological cells depend on it for sustenance. The new heterogeneous microstructure affects the way solutes diffuse through the gel and the effect is nonlinear. The scale of the structure is much smaller than the application scale, which prohibits direct simulation. We develop a method for two calcified hydrogels based on asymptotic homogenisation and show how the multiscale heterogeneities can be accounted for in a homogenised material model. The soon to be published results can be used to guide the production process and target specific material diffusivities.

On the effective electrical properties of microstructures featuring material interface

Dilek Güzel

TU Dortmund, Institut für Mechanik, Leonhard-Euler-Str. 5, 44227 Dortmund, Germany

Abstract The effective material response as observed at the macroscale is inherently related to the underlying microstructure and to lower-scale processes. Interfaces, such as phase and grain boundaries, significantly affect the overall material response, particularly in polycrystalline materials where grain boundaries act as notable sources of resistance, impacting electrical properties [1]. Computational multiscale formulations provide powerful approaches for capturing such distinct microscale processes and features.Motivated by the influence of grain boundaries on effective electrical properties, the computational multiscale framework for electrical conductors proposed in [2] is extended to continua with material interfaces at the microscale. Specifically speaking, (lowly-conducting) cohesive-type interfaces are considered at the microscale, such that displacement and electrical potential jumps across the interface can be accounted for. Averaging theorems for the field quantities are derived and consistency with the Hill-Mandel condition for suitable boundary conditions is shown. Size effects become particularly significant in materials with a high surface-to-volume ratio as is the case for nanoparticles or materials with a high density of interfaces like grain boundaries in polycrystalline materials. In contrast to the classic first-order homogenisation approaches, material interfaces at the microscale induce an internal characteristic length into the multiscale formulations [3]. As a result, the established framework allows the size-dependent material response due to the presence of material interfaces to be studied. To demonstrate the capabilities of the proposed framework, different representative simulations are selected and the size-dependent material response is systematically analysed. The simulation results are verified by means of quasi one-dimensional boundary value problems for which analytical solutions can be derived. Joint work with Tobias Kaiser and Andreas Menzel (TU Dortmund).

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Neural network propagators in data-driven inelasticity: An automated framework

Marius Harnisch

TU Dortmund, Institut für Mechanik, Leonhard-Euler-Str. 5, 44227 Dortmund, Germany

Abstract Data-driven mechanics, introduced by Kirchdoerfer and Ortiz [1], replaces conventional material modeling with data-sets containing snapshots of stress and strain assumed to be sufficiently accurate representations of the underlying material behavior. Build on these snapshots, denoted as material states, and on states fulfilling equilibrium and kinematic compatibility, called mechanical states, is a distance function, the minimization of which with respect to both the material and mechanical states yields the boundary value problems' solutions.

Originally introduced for elasticity, extending the framework to inelasticity presents a substantial challenge. Different approaches have been proposed in literature. We base our approach [2, 3] on a quantity denoted as history surrogate together with a propagator. By building our novel data-driven inelasticity framework on these quantities, we preserve the spirit of the elasticity approach and eliminate the necessity for real-time adjustments to the data-set. The history surrogate thereby stores essential information of the history of the material's response along the respective loading paths up to the current point in time and the propagator serves as an update rule at the end of each time step. This enables an offline definition of a fixed synthetic data-set for use in online data-driven simulations. While the challenge now shifts to defining a history surrogate both suitable and generally applicable – a complex task if tackled by hand – it also offers an outstanding opportunity: By utilizing a Neural Network as propagator [3], we allow for an autonomous framework, which extracts the essential information of the material's history without resorting to a material model. Such a model or modeling approach, is solely required when generating the raw input data in form of discrete paths of stress and strain. From there on, the Neural Network propagator allows for an automated framework, ranging from the construction of the data-set with a suitable history surrogate to the solution of boundary value problems with inelastic material behaviour – potentially allowing for the use of arbitrary user-defined material models in data-driven inelasticity, without the need of data-driven specific knowledge of the user.

In this contribution, we introduce our extension to inelasticity and highlight the capabilities of our novel approach. By presenting results for different inelastic processes utilizing a Neural Network propagator, we focus on the resulting automated framework such a Neural Network allows for. We show the necessary training routines of the network, discuss the obtained data-driven simulations and provide a comparison with an intuitive choice of history surrogate and propagator.

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[3] K. Poelstra, T. Bartel, B. Schweizer, A data-driven framework for evolutionary problems in solid mechanics, Z. Angew. Math. Mech. (103) (2023) e202100538

Anisotropic unified continuum model and 3D simulation for healing of damaged soft biological tissues

Yiqian He

Ruhr University Bochum, Institute of Mechanics of Materials, Thea-Universitätsstr. 150, 44801 Bochum, Germany

Abstract Computational modeling can provide an effective tool to simulate the healing process of soft biological tissues and understand underlying mechanism. In previous work, we developed a unified continuum damage model for the healing of soft biological tissues. However, our current results are still far from being generalizable to more realistic settings and applicable to realistic biomechanical problems because of the simplicity by isotropic constitutive model and two-dimensional simulation. In this article, we further develop a three-dimensional anisotropic unified healing model. By using Holzapfel-Gasser-Odgen model as the hyperelastic term, the influence of the collagen fibers is considered and the reorientation of fibers in healing can be simulated. Three numerical examples related to hypertension, aneurysm, and restenosis of the atherosclerotic artery after balloon angioplasty are provided to demonstrate the effectiveness of the proposed model.

Time-separated Stochastic Mechanics: A novel Approach for the Estimation of Random Fluctuations during Microstructure Evolution

Philipp Junker

Leibniz Universität Hannover, Institut für Kontinuumsmechanik, An der Universität 1, 30823 Garbsen, Germany

Abstract In recent work, we propose a novel technique to access the stochastic behavior of non-linear materials with randomly fluctuating properties. The related material models constitute ordinary differential equations with random coefficients which are well-known to be non-trivial to be analyzed. We develop a novel strategy for stochastic series expansion for such problems which allows us to separate the deterministic but time-dependent parts from the stochastic but time-invariant parts. Consequently, we referred this approach to as Time-Separated Stochastic Mechanics (TSM). Making use of this tailored stochastic series expansion, we are able to compute explicit formulas for all stochastic quantities, e.g., the expectation and standard deviation, for all physical state variables of interest, e.g., internal variables, stresses and reaction forces. From a practical perspective, the set of deterministic material parameters is extended which hence includes all necessary information on the stochasticity of the material behavior. The great advantage is that the numerical extra costs compared to standard deterministic computations are increased by only 10 to 30

In this talk, we present our recent advances on this promising new approach for the inclusion of stochasticity into the simulations of engineering constructions. This includes the investigation of different non-linear materials, e.g., viscoelasticity and phase transformations, and discuss the numerical implementation. We demonstrate the validity of our approach by comparisons to Monte Carlo simulations and showcase that we receive excellent agreement both for quasi-static and dynamic loading conditions at minimal numerical costs. Furthermore, we present that TSM functions for spatially homogeneous and inhomogeneous stochastic fields.

Joint work with Hendrik Geisler (Leibniz University Hannover) and Jan Nagel (TU Dortmund).

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Geisler H, Junker P.: Time-separated stochastic mechanics for the simulation of viscoelastic structures with local random material fluctuations, Comput. Methods Appl. Mech. Engrg., accepted for publication, 2023.

Microstructure Monitoring for Additive Manufacturing using Coupled Deep Neural Operators and Neural-Cellular-Automata

Shayan Kasiri Habibabadi

Technische Universität Braunschweig, Data-Driven Modeling of Mechanical Systems, Rebenring 64, 38106 Braunschweig, Germany

Abstract The process-structure-property relationship is crucial in determining the end product's material property in the field of additive manufacturing (AM). Achieving the desired material properties and process performance requires in-depth knowledge about how process parameters affect the material properties as well as having control over tuning those parameters for obtaining desired properties. Our goal is to improve this understanding by developing novel approaches to microstructure modeling and monitoring based on data-driven approaches. This is especially important when producing functionally graded materials, where variations in microstructure can be used to create materials with spatially varying properties. The methodology utilized in our study involves the implementation of an one-way coupling approach, which incorporates two state-of-the-art data-driven methodologies: Deep neural operators (DeepONets) and neural cellular automata (NCA). The initial stage of our methodology entails the reconstruction of the full-body temperature distribution, relying exclusively on surface temperature measurements. The consistent reconstruction of the temperature field is of great importance due to the significant influence of temperature on the creation of microstructures during the manufacturing process. The implementation of DeepONet enables reliable estimation of internal temperatures, a task that was previously challenging due to limitations in direct measurement. NCA offers an advanced method to simulate the evolution of microstructures in metals during solidification processes. This novel methodology integrates the fundamental concepts of cellular automata with the computational capabilities of neural networks, particularly convolutional neural networks (CNNs).

The integration approach described in this study demonstrates superior computational speed compared to standard methods, while maintaining a high level of accuracy. In summary, this study presents an innovative methodology that utilizes data-driven techniques for simulating microstructures in powder bed fusion (PBF) processes.The utilization of this technology enhances our capacity to predict and monitor the microstructure in PBF and may contribute to the fabrication of functionally graded materials.

Towards Concurrent Numerical Relaxation: Introducing an H-Sequence Based Algorithm for Concurrent Approximation of Rank-One Convex Envelopes

Maximilian Köhler

Ruhr University Bochum, Cintinuum Mechanics, Universitätsstr. 150, 44801 Bochum, Germany

Abstract Relaxation techniques stand as promising regularizations in various models owing to their unique characteristics: they introduce no additional length scale parameter and describe complex microstructures through semi-convex hulls. However, embedding concurrent numerical relaxation due to rank-one convexification within finite element simulations for incremental, dissipative models often incurs substantial numerical overhead, making it practical only in specific scenarios [1]. This talk introduces a novel algorithm leveraging hierarchical sequences (H-sequences) as a foundation, providing an equivalent characterization of the rank-one convex envelope [2, Definition 5.14]. The proposed method serves to approximate the rank-one convex envelope while offering an upper bound for it. Notably, for materials where each laminar level achieves energetic optimality concerning the current level, the approximated envelope aligns with the rank-one convex envelope. The study demonstrates applications in nonconvex finite strain continuum damage models (see [3]) in two and three dimensions, establishing a concurrent numerical relaxation for an incremental, dissipative large strain model. Crucially, this approach facilitates realistic finite element problem-solving by ensuring compatible microstructures. This presentation delves into various facets of the algorithm, encompassing the restoration of rotational invariance, microstructure reconstruction, comparisons with other semi-convex envelopes, and considerations regarding mesh dependency.

Joint work with Neumeier, Peter, Peterseim, Balzani.

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Material modeling of ferroelectricity enhanced by higher-order electromechanical coupling

Sergey Kozinov

Ruhr University Bochum, Continuum Mechanics, Universitätsstr. 150, 44801 Bochum, Germany

Abstract Flexoelectricity, a phenomenon that becomes increasingly pertinent at smaller scales, describes the intricate two-way interaction between strain gradients and electric fields. This phenomenon is of high importance in the design of micro- and nano-electromechanical systems, such as sensors, actuators, and energy harvesting devices, due to its enhanced effects at these scales. The current study addresses the innovative challenge of modeling ferroelectric materials while considering flexoelectricity. This task can be viewed from two angles: first, as a progression in ferroelectric modeling by incorporating higher-order electromechanical interactions, and second, as an expansion of flexoelectric modeling in dielectric and piezoelectric structures to include nonlinear material behavior. This dual perspective provides a thorough understanding of the interplay between ferroelectricity and flexoelectricity in intricate material systems. The study concentrates on developing constitutive relations for this advanced electromechanical coupling, utilizing the micromechanical switching model for ferroelectric polycrystals. The corresponding 3D numerical implementation advances the recently developed collocation-based mixed FEM and enhances the ferroelectric switching model with higher-order finite elements. The emphasis of these simulations is on examining the changes in ferroelectric polarization and strain hysteresis loops under flexoelectric influence.

Phase-field optimization, assessment, and experimental validation of minimal-surface micro-structures

Andreas Krischok

University of Stuttgart, Lehrstuhl für Materialtheorie, Pfaffenwaldring 7, 70569 Stuttgart, Germany

Abstract Inspired by lattice structures that are observable in nature, micro-porous materials have been causing an ever increasing interest in the recent years. This is not least due to the fact that the production of such materials becomes more and more feasible by means of additive manufacturing. In this regard, 3D-printed structures with graded volume fractions have been shown to provide superior properties in the context of providing an optimal compliance if subjected to non-homogeneous deformations but are likely to be inferior to optimized solids without a cell structure.

Since the optimal configuration of microscopic unit cells under heterogeneous macroscopic stress states will be nonlocal and anisotropic, one needs to design microstructures in a locally adaptive manner. We tackle this problem by means of a phase-field approach for the optimization of microstructures based on triply-periodic minimal surfaces. In that regard, it is out goal to obtain unit cells with a locally optimal homogenized stiffness with respect to the direction of the maximum principal stress. In the present contribution, we will show that different kinds of optimized microstructures exhibit fundamental differences with regard to their response to tension- or shear-dominated loads. Furthermore, we will discuss strategies to verify the gain of the stiffness response experimentally.

Joint work with Basavesh Yaraguntappa, Laurence Bodelot, Kostas Danas and Marc-Andre Keip.

Variational framework for damage modeling: Challenges and opportunities

Kai Langenfeld

TU Dortmund, Institut für Mechanik, Leonhard-Euler-Str. 5, 44227 Dortmund, Germany

Abstract Regularization methods are frequently applied to ill-posed models and damage models in particular. Typical limitations of ill-posed models include equivocality, a lack of differentiability, instability and – turning the view to the numerical implementation – a severe dependence on the mesh of the discretization. This is a clear obstacle for damage predictions that are critical for fail-safe operations and hazard-free environments. Regularization methods hence aim at turning the model descriptions into well-posed problems with reliable outcomes. Nowadays, several methods can be found in the literature for the regularization of ill-posed models, see e.g. [1, 2, 3]. Within the first part of this talk, the variational derivation of material models in terms of incremental energy minimization will be used as a unifying framework for the analytical and numerical comparison of the regularization methods [4]. The comparison focuses on (i) highlighting how wellposedness is achieved and (ii) the physics predicted by the regularized models. The second part of the talk will focus on the (micromorphic) gradient regularization [5]. In particular, the focus will be on an undesired side effect of this regularization technique: curvature dependence. This can become relevant in environments cracking with curved patterns such as crack initiation at smaller scales or tunnel lining [6]. The curvature dependence of the constitutive equations will be highlighted analytically and numerically. Subsequently, two approaches will be elaborated to control this curvature dependence and their extended properties will be demonstrated. It will be shown that the extended approaches allow to calibrate the curvature of the emerging crack without inducing additional affects on the underlying physics.

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Multi-scale numerical methods for reaction-diffusion equations with oscillating coefficients

Albéric Lefort

École Nationale des Ponts et Chaussées, 6-8 avenue Blaise Pascal, 77420 Champs-sur-Marne, France

Abstract We study theoretically and numerically multiple approaches for approximating the solution of the eigenvalue problem for the reaction-diffusion equation with oscillating coefficients:

$$\sigma_\epsilon u_\epsilon - \epsilon^2 \nabla.(A_\epsilon \nabla u_\epsilon) = \lambda_\epsilon u_\epsilon \qquad (1)$$

supplemented with homogeneous Dirichlet boundary conditions, and where $D_\epsilon = D(\frac{\cdot}{\epsilon})$, $\sigma_\epsilon = \sigma(\frac{\cdot}{\epsilon})$ are highly oscillating coefficients, assumed periodic for our theoretical results. The unknown is the couple $(u_\epsilon, \lambda_\epsilon)$ of the first eigenvector and eigenvalue for equation (1). This equation is especially used to model the neutron flux in a nuclear reactor core in a steady-state regime, where oscillating coefficients describe domain heterogeneity (with characteristic scale ϵ). As for multi-scale problems, numerical approximation of the solution by standard methods is too expensive. Here, we implement a numerical approach using the Multi-scale Finite Element Method (MsFEM), which is a Galerkin discretization approach using pre-computed basis functions that are well adapted to the problem of interest. Since these basis functions are solutions of local problems, the intricate task lies in finding the right local problems to solve. The advantage of this method relies upon the fact that once basis functions are pre-computed, the couple $(u_\epsilon, \lambda_\epsilon)$ can be obtained in a very short time. Moreover, the same basis functions can be used to efficiently derive any couple of eigenvalue/eigenvector of (1). We make partial use of theoretical homogenization results in a periodic framework to guide our intuition in order to define appropriate basis functions yielding an efficient approach.

Joint work with Claude Le Bris, Frédéric Legoll.

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Modeling wave propagation and boundary effects in acoustic metamaterials by a relaxed micromorphic continuum

Angela Madeo

TU Dortmund, Institute of Structural Mechanics and Dynamics, August-Schmidt-Str. 8, 44227 Dortmund, Germany

Abstract Exploring the dynamical response of mechanical metamaterials in the framework of elastic propagation has gathered increasing attention in the last decades. In order to describe elas- tic wave propagation in metamaterials, i.e. solids with heterogeneities or microstructure, it is necessary to consider non-local or enriched models. The relaxed micromorphic model (RMM) 2, 3] proposed here can describe these effects as a continuous material with enriched kine- matics. One of the most important micro-mechanical effects is the appearance of band gaps for which waves at given frequencies cannot propagate through the material. We have shown in previous papers [1, 2, 3] that the relaxed micromorphic model can describe the bulk behavior of mechanical metamaterials. Things become more complicated when consid- ering finite-size metamaterial blocks for which boundary effects may play a major role, e.g. due the reduced size of the block itself. In these cases, the relaxed micromorphic model frame- work must be enriched to account for these boundary effects. We will show how the concept of boundary forces can be used to address the modeling of finite-size metamaterial specimens in the context of micromorphic elasticity.

Joint work with Jendrik Voss, Svenja Hermann, Gianluca Rizzi, Felix Erel-Demore, Leonardo A. Perez Ramirez, Plastiras Demetriou and Patrizio Neff.

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Quasiconvex relaxation of a planar Biot-type energy with and without determinant constraints

Robert Martin

University Duisburg-Essen, Faculty of Mathematics, Thea-Leymann-Str. 9, 45127 Essen, Germany

Abstract We derive the quasiconvex relaxation of the Biot-type energy density $|U-1|^2$ for planar mappings in two different scenarios. First, we consider the case where the gradient of the mapping is constrained to the positive general linear group, in which case the energy can be expressed as the squared Euclidean distance to the special orthogonal group SO(2). We then allow for planar mappings with arbitrary deformation gradient; in the context of solid mechanics, this lack of determinant constraints on the deformation gradient would not exclude local self-interpenetration of matter. We demonstrate that the two resulting relaxations do not coincide and compare the analytical findings to numerical results for different relaxation approaches, including a rank-one sequential lamination algorithm, trust-region FEM calculations of representative microstructures and physics informed neuronal networks.

Computational Polyconvexification of Isotropic Functions

Timo Neumeier

Universität Augsburg , Angewandte Analysis / Numerische Mathematik, Universitätsstraße 12a, 86159 Augsburg, Germany

Abstract For the minimisation of energy functionals with non-convex energy densities that arise for example in pseudo-time-incremental damage models in the finite strain setting, polyconvex relaxation is a viable choice. However, the computational complexity of (semi-)convexification algorithms is heavily impacted by the computational dimension. As a consequence, direct finite element simulations on a larger scale are currently unfeasible when dealing with the d×d deformation gradient. To overcome this issue, we focus on the approximation of semi convex hulls for isotropic energy densities. The characterisation by means of the signed singular values leads to a feasible algorithm for the numerical approximation of the polyconvex envelope. Instead of operating on the dxd-dimensional space of matrices (the deformation gradient in typical applications), the algorithm requires only the computation of the lower convex envelope of a d-dimensional manifold. This is done using an optimisation approach or utilising standard computational geometry algorithms. A series of numerical experiments shows the substantial increase in computational speed resulting from the dimension reduction, when moving from full (d x d) matrix space to the space of signed singular values. This indicates the feasibility of the relaxation approach in finite element simulations for damage boundary value problems.

Joint work with Daniel Balzani, Maximilian Köhler, Malte A. Peter, Daniel Peterseim, David Wiedemann.

Morphology-Based Homogenization of Evolving Microstructures in Phase Transforming Solids

Vincent von Oertzen

TU Bergakademie Freiberg, Institute of Mechanics and Fluid Dynamics, Lampadiusstr. 4, 09599 Freiberg, Germany

Abstract The effective behavior of phase transforming materials directly depends on characteristic microscopic evolution processes—such as martensite reorientation, twinning, solidification or decomposition phenomena—during which the microstructure topology changes over time. A variety of important contributions have been made over the last decades to mathematically describe these multi-physical mechanisms, see [1,2] and the references therein. The majority of existing models relies on transient and spatially-regularized phase-field frameworks. Consequently, the embedding of existing routines into modern two-scale approaches, such as the FE2-method, is usually associated with enormous computational costs. The reason is that the involved temporal and spatial scales need to be resolved numerically with sufficient accuracy. Moreover, a general notion for consistently transferring specific phase-field models between multiple, variable scales has still not been fully developed.

To address these issues, the recently introduced concept of unequally and nonlinearly weighted averaging operators provides a promising homogenization framework [3]. Here, this rather general approach is used to macroscopically capture the evolution of laminate orientation in the dual-phase system ZrO2 that exhibits a displacive solid-solid phase transformation. It is mathematically demonstrated that macroscopic driving forces as well as effective mechanical properties can be expressed as functions of the average martensite volume fraction and, additionally, of a finite collection of weighted phase averages, so-called phase-morphologies. The effective evolution of martensite can therefore be determined through a macroscopic system of ordinary differential equations, which results as the homogenized response to a spatially regularized, microscopic phase-field model. In this regard, the validity of the outlined homogenization approach is demonstrated in two-dimensional finite element simulations of microstructure formation for various temperature- and strain-controlled loading scenarios.

Joint work with Bjoern Kiefer.

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Variational quantitative phase-field modeling and simulation of powder bed fusion additive manufacturing

Timileyin David Oyedeji

TU Darmstadt, Institute of Materials Science, Schlossgartenstr. 7, 64289 Darmstadt, Germany

Abstract Phase-field model has been proven to be a powerful tool in describing the complex porestructure evolution and the intricate multi-physics in powder bed fusion additive manufacturing process [1, 2, 3]. However, as one of the diffuse-interface approaches, the models employ a finite interface width in representing the transient microstructure. They have to be projected asymptotically onto their corresponding sharp-interface equations to guarantee their quantitative validity. Even though this issue has been solved for liquid-solid interfaces via the development of the quantitative solidification phase-field model [4, 5], there is no related work addressing the interfaces in powder bed fusion. In this work, we developed a variational quantitative phase-field model to overcome the issues of quantitative validity in powder bed fusion simulations. The model eliminates artificial interface effects caused by the diffuse-interface description of the interfaces, regardless of the finite interface width. Moreover, the model is derived in a variational manner and consistent with non-equilibrium thermodynamics. Cross-coupling terms between the conserved kinetics (i.e., mass and thermal transfer) and the non-conserved one (grain growth), which are typically neglected in conventional models, are considered in the evolution equations. These cross-couplings derived in terms of phase-field parameters via asymptotic analysis are instrumental in ensuring the elimination of interface effects. Furthermore, to enforce the quantitative validity of the model, it is apparent that anisotropic interpolation of the kinetic mobilities is essential. Numerically, we demonstrate the importance of the cross-couplings and the anisotropic interpolations, obtaining good convergence of results with respect to interface width. Also, we make comparisons of the microstructural results obtained using the model to the ones obtained via existing models.

Joint work with Yangyiwei Yang (TU Darmstadt), Herbert Egger (University Linz), Bai-Xiang Xu (TU Darmstadt).

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Linking Energy to Irregularity in Prestrained Elastic Sheets

David Padilla-Garza

TU Dresden, Institut für Wissenschaftliches Rechnen, Zellescher Weg 25, 01069 Dresden , Germany

Abstract This talk will delve into the link between prestrain regularity and energy in non-Euclidean thin elastic sheets. We show that in 2d stretching+bending models, prestrain irregularity implies a lower bound on the energy of the system. We also analyze the example of incompatible inclusions, a problem with applications in thin nematic elastomer sheets. In this example, we show a lower bound for general 3d elastic energy functionals and a matching upper bound, constructed by a combination of origami maps and Brehm isometries.

Phase-field modeling of domain switching in ferroelectric materials in the presence of a crack.

Thuc Pham Phu

Ruhr University Bochum, Cintinuum Mechanics, Universitätsstr. 150, 44801 Bochum, Germany

Abstract Ferroelectric materials are a subclass of piezoelectric materials that retain their polarization state below the Curie temperature after the applied electric field has been removed. The multi-field coupling between mechanical strain, and electric potential and polarization has caused these materials to rise in popularity in both industries and academia due to their wide range of application in sensors, actuators, and electronics. This study presents the phase-field model to describe the coupling phenomenon and the derived two-dimensional finite element implemented in ABAQUS UEL. The finite element subroutine is first validated by replicating results from several papers. Then, the polarization switching in ferroelectric specimens containing defects, such as cracks, voids, and notches was investigated. Subsequently, the contribution of polarization gradient terms in the phase-field equation to switching and domain pattern formation is explored and discussed.

Boundary Layer Estimates in Stochastic Homogenization

Claudia Raithel

TU Dresden, Institut für Wissenschaftliches Rechnen, Zellescher Weg 25, 01069 Dresden , Germany

Abstract We consider the quantitative stochastic homogenization of linear elliptic operators on the half-space. In particular, we obtain optimal decay rates (away from the boundary) for the correction of the whole-space corrector. As an application of our decay rates, we show how to obtain optimal convergence rates for the RVE method for approximating the homogenized coefficients (without the presence of a screening term).

On Scaling Laws for Some Microstructures in Shape-Memory Alloys

Angkana Rüland

Universität Bonn, Institut für Angewandte Mathematik, Endenicher Allee 60, 53115 Bonn, Germany

Abstract Shape-memory alloys display a rich energy landscape. In this talk, I discuss scaling laws for selected singular perturbation models for these materials. I discuss both upper and lower bounds.

Construction of coarse approximations for a Schrödinger problem with highly oscillatory coeffcient

Simon Ruget

École Nationale des Ponts et Chaussées, 6-8 avenue Blaise Pascal, 74420 Marne-La-Vallée, France

Abstract This presentation deals with inverse problems in a multi-scale context. Broadly speaking, the aim is to reconstruct the unknown coeffcient of an elliptic PDE involving several scales of interest. For a given problem, we propose to reconstruct some characteristic quantites associated to the PDE, based on the knowledge of solutions. Typically, these quantites are inspired by homogenization theory (e.g. effective coeffcient, corrector). The idea is to develop a numerical methodology that can handle cases beyond those traditionally considered by the homogenization theory (which have to satisfy assumptions that can be restrictive in practice (e.g. periodicity)), and that can be valid even outside the specific case where scales are well separated.

Joint work with Claude Le Bris and Frédéric Legoll.

Modeling and numerical analysis of antiferromagnetic and ferrimagnetic materials

Michele Ruggeri

University of Bologna, Department of Mathematics, Piazza di Porta San Donato 5, 40126 Bologna, Italy

Abstract We consider the numerical approximation of a continuum model of antiferromagnetic and ferrimagnetic materials. The state of the material is described in terms of two unit-length vector fields, which can be interpreted as the magnetizations averaging the spins of two sublattices. For the static setting, which requires the solution of a constrained energy minimization problem, we introduce a discretization based on first-order finite elements and prove its Γ-convergence. Then, we discuss iterative algorithms for the computation of low-energy stationary points. Finally, we extend the algorithms to the dynamic setting, and we prove unconditional stability and convergence of the finite element approximations toward a weak solution of the problem. Numerical experiments assess the performance of the algorithms and demonstrate their applicability for the simulation of physical processes involving antiferromagnetic and ferrimagnetic materials. This is joint work with Hywel Normington (University of Strathclyde).

Hywel Normington, Michele Ruggeri: Convergent finite element methods for antiferromagnetic and ferrimagnetic materials. arXiv:2312.04939 (2023).

Parametrized balanced-viscosity solutions to a rate-independent hydraulic fracture model

Viktor Shcherbakov

University of Kassel, Institute of Mathematics, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

Abstract A hydraulic fracture refers to the phenomenon of pressure-induced fractures propagating in solid media under the injection of fluid. In this talk, we adhere to the philosophy of rate-independent systems to discuss, within the small-strain setting, a sharp-crack evolution model for the hydraulic fracture that is based on local minimizers and allows for free, but regular paths. The fracture evolution is driven by a global volume conservation law postulating that a total injected volume of incompressible fluid coincides with the fracture volume. We establish the existence of parametrized balanced-viscosity solutions to the model. The talk is based on a joint work with Dorothee Knees (University of Kassel) and Victor Kovtunenko (University of Graz).

Kinematics of micromorphic continua and suitable finite element spaces

Adam Sky

University of Luxembourg, Institute of Computational Engineering and Sciences, 6 Avenue de la Fonte, L-4362 Esch-sur-Alzette, Luxembourg

Abstract Micromorphic continua is a general name for every continuum model with an enriched kinematic of the material point. The full micromorphic model is known as the Eringen-Mindlin model, which assumes the complete gradient of the microdistortion field DP , contributes to the energy functional of the formulation. Seting the microdistortion to be equal to the gradient of the displacement field in the latier P = Du, yields the model of gradient elasticity. Assuming only the skew-symmetric part of the gradient of the microdistortion contributes to the energy relates the Eringen-Mindlin model to the relaxed micromorphic model, where the Curl is employed instead of the full gradient Curl P . The relaxed micromorphic model allows to even further weaken the control over P by employing sym Curl P in the energy functional. Each one of the latier choices imbues the micromorphic model with a set of possible kinematics, and determines the capacity to relate it to precise materia, such as metamaterials. Further, these choices and the arising kinematics must be directly accommodated by the finite element discretisation. In this talk we discuss the possible kinematics of the models, their appropriateness for material modelling, and suitable finite element spaces for their computation.

Joint work with A. Zilian (University of Luxembourg) and P. Neff (University of Duisburg-Essen).

Modelling Abscission of Plant Organs as Inspiration for the Separation of Materials Artificial Systems

Ludwig Striet

Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, Hermann-Herder-Str. 10, Raum 212, 79104 Freiburg im Breisgau, Germany

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

Modeling microstructural effects in scaffold mediated bone regeneration

Oliver Suchan

Albert-Ludwigs-Universität Freiburg, Abteilung für Angewandte Mathematik, Hermann-Herder-Str. 10, Raum 212, 79104 Freiburg im Breisgau, Germany

Abstract When bone defects of large size occur, also called critical defects, the regenerating bone tissue is not able to bridge the resulting gap on its own and an additional artificial structure is necessary to support bone growth. We present a general framework to phenomenologically model the growth of bone mediated by such a scaffolding structure. The microstructural geometry and the porosity of the implemented structure have a significant impact on the bone growth rate which we seek to maximize by means of PDE constrained optimization. To also account for the microstructure we use periodic homogenization at each point of the macro space. Implemented within the firedrake framework, External Operators enable us to perform this micro-macro coupling with differing approaches for solving the micro and macro problems respectively. Here, we present the classical FE^2-method and compare it to a faster FE-FFT-approach.

FE-FFT-based multiscale simulations of polycrystalline materials

Johanna Waimann

RWTH Aachen, Institut für Angewandte Mechanik, Mies-van-der-Rohe-Str. 1, 52074 Aachen, Germany

Abstract The behavior of a material is highly influenced by its microstructure. In order to use a material resource-efficiently, it is important to know its behavior as precisely as possible and to be able to simulate it in a time-efficient manner. To capture complex local microstructural effects such as phase transformations or crystal plasticity, we present a two-scale approach which utilizes a finite element (FE) formulation at the macroscale and a fast Fourier transformation (FFT)-based description at the microscale [1, 2]. We would like to present the two-scale method's ability to model highly resolved thermo-mechanically coupled problems and its application in the field of microstructural evolutions in polycrystalline materials, e.g. [4]. An additional focus of our presentation is on the introduction of model order reduction techniques. We propose an approach, which is based on an adaptively chosen reduced set of Fourier modes [3] and thus decreases the high computational costs of the FFT-based microstructure simulation.

Joint work with Christian Gierden (RWTH Aachen University), Annika Schmidt (RWTH Aachen University) and Stefanie Reese (University of Siegen).

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Homogenisation of a system of Stokes flow and advection–reaction–diffusion transport in a porous medium with coupled evolving microstructure

David Wiedemann

TU Dortmund, Angewandte Analysis, Vogelpothsweg 87, 44227 Dortmund, Germany

Abstract We consider the homogenisation of the Stokes equations and an advection–reaction–diffusion equation in an porous medium with evolving microstructure. The microstructure's evolution is coupled with the unknown concentration resulting in a free boundary value problem. We transform the problem on a fixed periodic domain, which results in a non-linear problem. By homogenising this substitute problem and transforming the limit problem back, we obtain as effective limit problem a Darcy law for evolving microstructure coupled with advective–reactive–diffusive transport.

Joint work with Markus Gahn, Malte A. Peter, Iulio Sorin Pop.