GAMM 2023

22nd GAMM Seminar on Microstructures

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Organizers of the Young Researchers Meeting:
Lorenza D'Elia (TU Wien),
Valerio Pagliari (TU Wien)

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Invited Speakers

Modeling and Simulation of Thin Sheet Folding

Sören Bartels, Universität Freiburg

Joint work with Andrea Bonito, Peter Hornung and Philipp Tscherner.

The folding of a thin elastic sheet along a curved arc has various applications including the construction of bistable devices. We discuss the derivation of a plate model from three-dimensional hyperelasticity and rigidity properties of admissible deformations and minimizers. The numerical solution is based on an isoparametric discontinuous Galerkin finite element method that provides a suitable geometric approximation of the folding arc. Error estimates are presented for a linearized version of the model problem.

3D variational models for dislocations

Roberta Marziani, TU Dortmund

Dislocations are line-defects in crystals caused by the plastic slip of layers of atoms over each other. In this talk, we give a brief introduction on theory of dislocations in the context of continuum elasticity. Afterwards we will consider a 3-dimensional variational model for dislocations. In particular, we show that the asymptotics via Gamma-convergence is independent of the specific choice of the energy and of the regularization procedure. This result is based on a recent result obtained in collaboration with Sergio Conti and Adriana Garroni.

On the localization problem in numerical deterministic and stochastic homogenization

Daniel Peterseim, Universität Augsburg

Numerical homogenization aims to effectively approximate solution operators of partial differential equations (PDEs) with heterogeneous coefficients by the choice of problem-adapted approximation spaces. Uniform convergence rates are theoretically achieved for arbitrarily rough PDE coefficients by applying the solution operator to some standard finite element space. However, the canonical basis associated with this construction is non-local and, therefore, numerically intractable. This is why the true challenge of numerical homogenization is the identification of a computable local basis for such an operator-dependent approximation space. This talk presents a near-optimal constructive solution to this so-called localization problem for prototypical linear deterministic and random elliptic operators. A sequence of numerical experiments illustrates the significance of the method for the simulation of physical processes beyond classical homogenization problems.

Random microstructure and stochastic homogenization

Matthias Ruf, EPFL

We present the probabilistic framework for environments with random oscillations on a microscale that look statistically homogenous on large scales. We then discuss several variational models and present results on the asymptotic behavior when the scale of the oscillations tends to zero. If time permits, we also discuss the basic elements of the proofs.

Model-free Data-driven Paradigms for Multi-scale Mechanics

Laurent Stainier, Centrale Nantes

Nowadays, it has become relatively common to construct numerical material models, relying on a description of constitutive response and architecture at the finer scales (atomistic, microscopic, ...). These numerical models provide abundant information on the global and local response, including interactions between the various components of the material, to given macroscopic loadings. The process of scale transition, consisting of identifying an effective macroscopic response, nonetheless remains a bottleneck. Indeed, an explicit representation of this response through a macroscopic constitutive model is not always (and actually seldom) easy nor appropriate, while an implicit representation by the complete numerical model (e.g. FE2) leads to an excessive computational cost. A popular alternative is to use meta-models, specially those based on deep-learning, but this approach comes with its own limitations: absence of interpretability, unknown extrapolation capability, lack of mathematical analysis (convergence, ...).
In this contribution, we will present how the (macroscopic) model-free data-driven approach proposed by Kirchdoerfer and Ortiz can be adopted to optimally exploit data generated by numerical material models. In particular, we will discuss alternative approaches aiming at constructing a goal-oriented database, optimally using the numerical material model and significantly improving computational efficiency of multiscale simulations.

A combined Filtered/phase-field approach to topology optimization in elasticity

Ulisse Stefanelli, Universität Wien

I will present a combined filtered/phase-field approach to topology optimization in the setting of linearized elasticity. Existence of minimizers, rigorous parameter asymptotics, and the convergence of an abstract space discretization in the spirit of conformal finite elements will be tackled by means of variational techniques. This is joint work with Ferdinando Auricchio (Pavia), Michele Marino (Rome Tor Vergata), and Idriss Mazari (Paris Dauphine).

Geometry of needle-like microstructures in shape-memory alloys

Barbara Zwicknagl, HU Berlin

Needle-like microstructures are often observed experimentally near macro-interfaces in shape memory alloys. The geometry of a needle-like domain is mainly characterised by its tapering length and the bending angle at the interface. Mathematically, such patterns are usually modelled in the framework of the phenomenological theory of martensite. The latter is based on finite or geometrically linearized elasticity. The focus of this talk lies on the tapering length of the needle. We discuss recent analytical and numerical results on the scaling of the minimal energy in terms of the tapering length, both in finite and linearized elasticity. This talk is based on joint works with S. Conti, M. Lenz, N. Lüthen, M. Rumpf, and J. Verhülsdonk.

Contributed Talks

The effect of pore-wall morphology on the scaling exponents for open-porous materials

Shivangi Aney, DLR Köln

Shivangi Aney[1], Ameya Rege[1,2], Lorenz Ratke[1,3], Barbara Milow[1,3]
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Open-porous materials such as aerogels are characterized by a network of pores which have a significant influence on the material properties. For example, in case of cellular materials, the influence of the pore sizes and the pore-size distributions has been investigated, both theoretically and computationally [1,2]. In these approaches, the pore walls were modelled as beams with constant cross-section. While this assumption is sufficient for cellular materials with fibrillar morphology, it seems too ideal for particle-aggregated materials which possess a pore-wall structure similar to a chain of pearls. It has been observed that approximating the pore-wall of such materials with a constant cross-section can lead to serious miscalculations of their mechanical behavior [3]. Thus, the effect of the pore-wall morphology is studied further using the Gibson and Ashby power law relation [4, 5] which correlates the relative density of the material with its Young's Modulus. In this contribution, unit cells with different pore-wall structures are created. These structures are simulated under compressive loads to calculate the respective scaling exponents. It has been shown that while the pore-wall morphology plays an important role in the prediction of the failure of the material, its influence on the scaling exponents is not comparable.

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Hybrid high-order methods (HHO) for nonlinear problems?

Carsten Carstensen, HU Berlin

C. Carstensen (HU Berlin) and N.T. Tran (U Jena)

The novel methodology of skeletal schemes led to a new generation of nonstandard discretisations and HHO [2,4] is one of many of those besides HDG, VEM, DPG, et al. that generalize naturally to nonlinear problems. Can a variational crime lead to discretisations superior to conforming ones? The key for the success of higher-order schemes is through adaptive mesh-refining and the basis of this is a reliable and efficient a posteriori error analysis. The later is a topic in its infancy at least for HHO [4]. While over-stabilization enables some progress for DG and VEM, it is a refined analysis [3] that makes a stabilization-free a posteriori error estimate possible for the HHO [1].

The application of an unstabilized HHO method to the class of degenerate convex minimization problems with two-sided growth conditions and an appropriate convexity control [7] leads to guaranteed error control [8] with a convergent adaptive mesh-refinement algorithm [9] for the dual stress-type variable.

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A phase field model for ferroelectrics with nonlinear kinetics and electro-mechanical coupling

Hsu-Cheng Cheng, ETH Zürich

Phase field modeling has been widely applied to model the evolution of domain patterns in various phase transformation problems. Existing phase-field models for the evolution of domain structures in ferroelectrics are based on an Allen-Cahn-type evolution law. However, this evolution law, which assumes a linear kinetic relation between the thermodynamic driving force acting on a domain wall and the domain wall velocity, fails to capture rate effects in ferroelectrics. To overcome this limitation, we propose a new phase field model for ferroelectrics (Guin, et.al , 2022), one that incorporates nonlinearities in the kinetics of domain walls and fully accounts for electro-mechanical coupling. As a multi-phase-field generalization of the model of Alber and Zhu (2013), it is based on the domain volume fraction of each variant as the primary phase field and incorporates the anisotropic dielectric, elastic, and piezoelectric properties of the different variants. With the ability to easily modify these different material properties, we investigate the relative contributions of electrostatics, mechanics, and piezoelectric effects to the motion of domain walls. The phase field model is validated through a comparison with the target sharp-interface model embedding nonlinear kinetics. Finally, limitations regarding the need to incorporate a separate nucleation process and open challenges (in common with all ferroelectric phase field models) with respect to the magnitude of the interfacial energy of domain walls are discussed.

Finite-strain Poynting-Thomson model: existence and linearization

Andrea Chiesa, Universität Wien

We investigate a large-strain Poynting-Thomson rheological model of viscoelastic materials. Here the total deformation is defined as the composition of a compatible viscous deformation and an elastic one, in accordance with the classical multiplicative decomposition of the total strain. We follow a time-discretization approach based on incremental minimization and prove the convergence of discrete solutions. Moreover, we study the linearization of the model showing convergence to the small-strain limit.

Asymptotic variational analysis of single-crystal plasticity in the limit of vanishing thickness and rigid elasticity

Dominik Engl, KU Eichstätt-Ingolstadt

We derive, with the help of Gamma-convergence, one-dimensional string theories from two-dimensional single-slip finite plasticity models under the assumption of rigid elasticity. In particular, we show that limit deformations can essentially freely bend even if subjected to the most restrictive constraints corresponding to the elastically rigid single-slip regime. The primary challenge arises in the upper bound, where the differential constraints render any bending without incurring an additional energy cost particularly difficult. We overcome this obstacle with suitable non-smooth constructions and prove that a Lavrentiev phenomenon occurs if we artificially restrict our model to smooth deformations. This issue is absent if the differential constraints are appropriately softened. This is joint work with Stefan Krömer and Martin Kružík.

Scaling Laws and the Emergence of Complex Patterns in Helimagnetism

Janusz Ginster, HU Berlin

In this talk we discuss a variational approach to study pattern formation in Helimagnets. After a brief introduction to the technique of scaling laws, we turn our attention to studying the emergence of patterns in magnetic compounds near the helimagnetic/ferromagnetic transition point in case of incompatible Dirichlet boundary conditions for the spin field. The energy under investigation is a continuum approximation of a J1-J3-model. It contains three parameters, the first measuring the incompatibility of the boundary conditions, the second measuring the cost of changes between different chiralities and the third depends on different optimal angle velocities of the spin field in rows and columns. We prove a scaling law for the minimal energy in terms of these parameters. The constructions from the upper bound indicate that in some regimes branching-type patterns form close to the boundary of the sample. Eventually, we discuss how the results in the continuous setting can be transferred to the discrete J1-J3-model.
Joint work with Melanie Koser and Barbara Zwicknagl (both Humboldt-Universität zu Berlin, Germany).

Derivation of a Bending Theory for Nematic Liquid-Crystal Elastomeric Plates through Gamma-Convergence

Max Griehl, TU Dresden

Liquid-crystal elastomers (LCEs) are materials whose shape can be controlled via external stimulation thanks to liquid crystal structures inside of polymer chain networks. To describe the deformation and microscopic liquid-crystal behavior of these materials, we start from a three-dimensional model taking into account coupled terms of hyper-elasticity and Oseen-Frank-type energy. Using Gamma-convergence, we then derive a dimension-reduced model, effectively describing thin LCE-plates in terms of a deformation and a liquid-crystal director field. We also take into account different types of boundary conditions for the deformation and the director field during Gamma-convergence.

On a modular data-driven framework for inelastic material behavior using history surrogates

Marius Harnisch, TU Dortmund

The data-driven mechanics, introduced in 2016 by Kirchdoerfer and Ortiz, is a method in the field of computational mechanics, which replaces conventional material models with data sets containing matching pairs of stresses and strains. The solution of the boundary value problem is based on minimizing a distance between states within these data sets, referred to as material states, and states satisfying equilibrium conditions and kinematic compatibility, referred to as mechanical states. Current research in this area addresses the challenging task of extending the method to account for path-dependent material behavior. In this contribution, we present a novel approach to tackle this task by the extension in terms of two quantities: A history surrogate, that stores essential information on the history of the material up to the current point in time and an associated propagator that serves as an update rule.

One distinctive feature of our approach is that these quantities are used as substitutable modules that affect both data generation and data-driven simulation. In detail, the framework consists of six modules: The first one is defined by the raw input data, i.e. the paths of discrete stress-strain pairs which contain the information of the materials behavior to be depicted. The suitable history surrogate is defined in the second module and updated via the propagator, which, although closely related to the history surrogate, represents a separate third module. Both previous modules are utilized in the fourth module to construct a data set. The data-driven solver, being the fifth module, uses this data set to calculate a physically admissible solution to the given boundary value problem. Lastly, the search algorithm for the determination of the current material states represents the sixth module. Due to this modularity, the structure of the original approach is maintained, thereby allowing for a straightforward extension of existing codes for elasticity.

In addition to the possibility of an intuitive definition, which may only apply to specific cases, a universally applicable approach is a Neural Network as history surrogate and propagator. The resulting framework is able to find a suitable history surrogate and perform data-driven simulations of inelastic material behavior solely based on the raw input data. On this basis, we highlight the capabilities of our novel approach by presenting results of different inelastic processes, e.g. plasticity and phase transformations in shape memory alloys, different non-monotonic loading paths, and different solvers, e.g. a staggered and a MIQP solver.

Advances in Relaxed Continuum Damage Mechanics at Finite Strains: Adaptive Convexification and Strain Softening

Maximilian Köhler, Timo Neumeier, Malte A. Peter, Daniel Peterseim, Daniel Balzani

In this talk, we will present recent work in the modeling of strain softening as a partially evolving microstructure, which is mathematically described by a successive decrease of the slope of the convex hull. This convex hull is constructed as homogenization of an evolving microstructure consisting of strongly and weakly damaged phases. In contrast to previous approaches, the model allows the strongly damaged phase to evolve itself in terms of an elastic unloading, which fixates the associated internal variable of this phase. This requires new convexification in each incremental time step and thus, the approach is referred to as reconvexification. Thereby, it has the capabilities to describe strain- and stress-softening in relaxed damage modeling at finite strains. We have developed efficient and adaptive convexification strategies for one-dimensional cases, which are used as integral part of a microsphere-based formulation to obtain the three-dimensional response using the reconvexified energy. In numerical benchmark problems, the proposed approach is shown to allow for mesh-independent calculations while enabling a realistic representation of strain-softening in e.g., soft biological tissues.

Controlled Cracking for Strain Relief in Highly Stretchable Multi-Layer Polymer Structures

Phillipp Kowol, Universität Wuppertal

Stretchable electronics exploit the characteristics of soft biocompatible polymers and utilize microstructural designs to push the boundaries of brittle conductor materials. A novel approach aims to increase macroscopic stretchability by introduction of controlled cracks in the polymer substrate's surface [1]. The cracks are deliberately induced by a micropattern of soft island crack starters in the hardened surface. Here, we study crack evolution in dependence of the micropattern design using numerical modeling [2]. A cohesive zone is used to capture the fracture behavior in the soft and hardened PDMS parts of a fully parameterized representative volume element [3]. We investigate the mechanical behavior of the layered polymer substrate and consider the influence of different material and geometry properties, e.g. ratio of Young's moduli, hardened layer thickness, or distance between cracks. The results show that cracks and soft islands accommodate the majority of the applied macroscopic strain while the hardened surface remains mostly strain-free, indicating that electronic devices or metal thin films could be applied with minimal risk of damage. Moreover, the simulations reveal interactions between parameters, which allows to identify design principles for large usable surfaces on polymer substrates utilizing controlled cracking.

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The variational approch to supercritical fractional perimeter (s>1) and to the s-fractional heat flow and the limit cases s go to 0 and 1.

Andrea Kubin, TU München

We consider a core-radius approach to nonlocal perimeters governed by isotropic kernels having critical and supercritical exponents, extending the nowadays classical notion of s-fractional perimeter, defined for $0 < s < 1$, to the case s>1.

In the second part of the talk, we prove that s -fractional heat flows converge to the standard heat flow as s go to 1, and to a degenerate ODE type flow as s go to 0.

L1-Korn-Maxwell-Sobolev inequalities in all dimensions

Peter Lewintan, Universität Duisburg-Essen

We characterize all linear part maps A[.] (e.g. A=sym) which may appear on the right hand side of Korn-Maxwell-Sobolev inequalities for incompatible tensor fields P. The correction term Curl P appears thereby in the L1 norm on the right hand side. Different from previous contributions, the results gathered in this work are applicable to all dimensions and optimal. This particularly necessitates the distinction of different constellations between the ellipticities of A and the underlying space dimensions n, especially requiring a finer analysis in the two-dimensional situation.
These results are based on a joint work with Franz Gmeineder (Konstanz) and Patrizio Neff (Essen).

Higher Dimensional Numerical Relaxation in Continuum Damage Mechanics

Timo Neumeier, Malte A. Peter, Daniel Peterseim (University of Augsburg),
Daniel Balzani, Maximilian Köhler (Ruhr-Universität Bochum)

In this talk, we focus on the simulation of a pseudo-time-incremental damage model in the finite strain setting. Due to the damage evolution, the incremental strain energy densities become non-convex and, thus, the direct numerical simulation suffers from mesh dependence and stability issues.
To overcome these drawbacks, we establish the relaxed model and discuss feasible algorithms for the approximation of semi-convex hulls, like the rank-one convex envelope, in higher spatial dimensions.
The use of weaker convexity notions enables the relaxed model to capture strain-softening of the material while providing mesh-independent approximations at the same time.

A homogenized bending theory for prestrained plates

David Padilla-Garza, TU Dresden

Nonlinear plate theory described the energy of an incompressible and inextensible thin elastic sheet. In this work, we show a general rigorous derivation of a generalization of such a model for non-euclidean plates with microheterogeneous structures. We also analyze the limiting energy in some examples and discover interesting and counter-intuitive phenomena.

Acoustic streaming in porous structures - homogenization based modelling

Eduard Rohan, University of West Bohemia

AUTHORS: Eduard Rohan and Fanny Moravcova

The acoustic streaming (AS) appears due to inhomogeneities in viscous flow inducing a non-zero divergence of the Reynolds stress (effects of kinetic energy of the velocity fluctuations), or due to vibrating fluid-solid interface (effects of surface acoustic waves). It is observed at fluid boundary layers as the Rayleigh streaming due to the viscous phenomena (low frequencies). This latter effect associated with the fluid-solid interface is in a sense amplified in periodic scaffolds. Applications in microfluidics and metamaterial design are challenging. We derive the homogenized model of the AS phenomenon within the framework of the classical perturbation approach which enables to linearize the Navier-Stokes (N-S) equations governing the barotropic viscous fluid dynamics in pores in a rigid periodic structure. The obtained first (P1) and second order (P2) sub-problems are treated by the asymptotic homogenization to derive the macroscopic model of the porous medium describing the AS phenomenon. Both the homogenized sub-problems P1 and P2 involve the same dynamic permeability. The P1 describes the acoustic waves in the homogenized pore fluid. The time averaged wave response provides a driving force (through the divergence of the Reynolds stress) for the P2 problem; its solution describes a steady flow at both macro- and micro-levels. The paper focuses on analytical and numerical methods developed to solve efficiently the acoustic streaming problem in the homogenized porous medium. An extension for elastic scaffolds is outlined.

Generalised bounded deformation on Riemannian manifolds

Emanuele Tasso, TU Wien

In the last decades the study of Free Discontinuity functionals has led to the development of different notions of functions with bounded variation. In an applied framework, the spaces GBV and GBD have been introduced to supply the lack of integrability of the field v and of the jump $[v]$ with respect to the $(n-1)$-dimensional Hausdorff measure $\mathcal{H}^{n-1}$ restricted to the jump set J_v. The spaces GBD and $GSBD$, in particular, have found applications in the study of functionals of the form

$$\int_\Omega |\tilde{e}(v)|^2 \,\mathrm{d}x + \mathcal{H}^{n-1}(J_v)\,, \tag{0.1}$$

where $\tilde{e}(v)$ denotes the approximate symmetric gradient of v. When dealing however with thin structure, like the case of a linearly elastic shell, namely, a 2-dimennsional regular surface in $\mathbb{R}^3$,

one is lead to the study of energy functional of the form

$$\int_{\omega} |e(u)|^2 \,\mathrm{d}x + \mathcal{H}^{n-1}(J_u), \tag{0.2}$$

where $\omega \subset \mathbb{R}^2$ is an open set and $e(u)$ is the *curvilinear symmetric gradient* of $u\colon \omega \to \mathbb{R}^2$. For instance, if the shell is parametrized by a map $\phi\colon \omega \to \mathbb{R}^3$ the curvilinear symmetric gradient of u is a 2×2 symmetric matrix defined as

$$2[e(u)]_{ij} := \partial_i u_j + \partial_j u_i - 2\sum_{\ell=1}^{2} u_\ell \Gamma_{ij}^{\ell}, \qquad i,j = 1,2,$$

where Γ_{ij}^{ℓ} denote the Christoffel symbols induced by ϕ.

With this motivation, in this talk I will introduce $GBD(M)$, namely, the space of functions with generalised bounded deformation on a Riemannian manifold M. The definition is given as in the euclidean case via slicing. However, the non-linearity of the ambient space introduces new difficulties which we will be able to circumvent with the introduction of new techniques. In particular, we will see that the jump set of every $u \in GBD(M)$ can be reconstructed by means of the jump sets of its one dimensional slicing and that u admits a.e. an approximate symmetric gradient $\tilde{e}(u)$. By means of $\tilde{e}(u)$ it is possible to define the approximate curvilinear symmetric gradient $e(u)$ of u, which is exactly the term appearing in the bulk energy part of (0.2). Eventually, if time permits, we will discuss how the above mentioned structure properties play a fundamental role in studying compactness and lower semicontinuity of the spaces $GBD(M)$ and $GSBD(M)$.

On scaling properties for two-state problems

Camillo Tissot, Universität Heidelberg

We study quantitative rigidity properties for the compatible and incompatible two-state problems for suitable classes of A-free operators. In particular, in the compatible setting we prove that all homogeneous, first order, linear operators with affine boundary data which enforce oscillations yield the typical epsilon-2/3-lower scaling bounds. As observed by Chan and Conti [CC15] for higher order operators this may no longer be the case. Revisiting the example from Chan and Conti, we show that this is reflected in the structure of the associated symbols and that this can be exploited for a new Fourier based proof of the lower scaling bound. Moreover, we highlight the relevance of the divergence operator as a prototypical example.

Asymptotic analysis of a family of non-local functional on sets

Andrea Torricelli, University of Modena / Reggio Emilia

We study the asymptotic behavior of a family of functionals which penalize a short-range interaction of convolution type between a finite perimeter set and its complement. We first compute the pointwise limit and we obtain a lower estimate on more regulars sets.

Homogenization of nonlinear randomly perforated materials under minimal assumptions on the geometry

Konstantinos Zemas, Universität Münster

In this work we combine and generalize earlier works of Giunti-Höfer-Velazquez (on the homogenization of the Poisson equation in random critically perforated domains) and Ansini-Braides (on a variational approach for the more general nonlinear vectorial problem in the periodic setting), each one in the direction of the other.
Namely, we show that under similar general assumptions on the geometry of the random perforations as the ones posed in the work of Giunti-Höfer and Velazquez, the stochastic analogue of the result of Ansini-Braides holds true, with an average deterministic nonlinear capacitary-term appearing in the Γ-limit.
This is joint, ongoing work with Caterina Zeppieri and Lucia Scardia.

Anisotropic Acoustic Waves In Diluted Nematic Liquid Crystals

Umberto Zerbinati, University of Oxford

Nematic liquid crystals are anisotropic elastic fluids. Such anisotropic behaviour stems from the orientation of the molecules composing the liquid crystal. In this talk, we assume nematic liquid crystals are fluids made up of rod-like structures satisfying C.F. Curtiss kinetic theory for non-spherical molecules [1]. In particular, the balance laws obtained from the usual four collision invariants for the Boltzmann type equation proposed by Curtiss are recast in the form of the Ericksen-Leslie equations which instead are usually obtained from a continuum mechanics point of view. Then we make use of the particular shape for the Cauchy stress tensor obtained from this kinetic approach to derive a particular set of equations describing the propagation of acoustic waves in diluted nematic liquid crystal.

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