Almi, Stefano

Title: A phase-field approach to Topology Optimization in elastoplasticity

Abstract: Topology optimization aims at detecting the optimal distribution of a material within a fixed region with respect to given target functionals. We will present a phase-field approach to Topology Optimization for a time-evolving elastoplastic medium subjected to kinematic hardening. We will show the existence of optimal configurations and compute their first-order optimality conditions. For the latter, we will proceed by subsequent approximations. We indeed consider a time discretization and a regularization of the flow rule. In such framework, we are able to compute the first-order optimality conditions and study their unregularized time-continuous limit.

Bartel, Thorsten

Title: Relaxed energy potentials based on A-quasiconvexity: Application to shape memory alloys

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Abstract: The combined physically and mathematically sound modelling and simulation of the inelastic constitutive behaviour of heterogeneous materials is still a major challenge in continuum mechanics. In this context, the concept of quasiconvexification is not only a suitable mathematical tool to proof the existence of solutions. From the viewpoint of mechanics, it might also be regarded as the optimal homogenisation method. Being achievable only in rare cases, however, the quasiconvex energy hull of an underlying non-quasiconvex energy landscape (e.g. a multi-well potential) is approximated in terms of upper and lower bounds. The perturbations applied in order to achieve such bounds are commonly defined with respect to curl-free fields, e.g. deformation gradients derived from compatible displacement fields. Such approaches, for example in the context of laminate-based perturbation fields, a priori fulfil the Dirichlet-type as well as the Neumann-type continuity conditions at underlying interfaces. The drawback of this concept lies in the fact, that in general upper bounds to the quasiconvex hull are obtained. Thus, the effective energy potential may violate the Cauchy-Hadamard condition and numerical simulations may suffer from instabilities.

The concept of A-quasiconvexity according to Fonseca and Mueller [1999], however, provides a framework that still exhibits all of the aforementioned beneficial features, but approaches the quasiconvex hull from a different "side". More precisely speaking, divergence-free fields such as stresses are perturbed in order to find energetically favourable states. Thus, the related energy relaxation process shall yield a lower bound to the quasiconvex hull and the Cauchy-Hadamard condition shall be satisfied. In the present contribution, specific relaxed energy potentials are derived based on the perturbation of stress fields with the aim of finding laminate-based energy hulls that may preserve the beneficial features of quasiconvexity. The numerical examples will focus on simulations of the behaviour of shape memory alloys, where possible extensions in view of smart materials such as magnetic shape memory alloys will also be addressed.

References: Fonseca and Mueller [1999], A-quasiconvexity, lower semicontinuity, and Young measures, SIAM J. Math. Anal. 30(6), pp. 1355-1390, 1999

Brands, Dominik

Numerical investigation of residual stresses on multiple scales during the cooling of hot formed parts

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Key Words: Phase Transformation, Multiscale Computation, Residual Stresses

The improvement of components properties, e.g. life time or strength, is a major objective in todays research. Considering hot forming processes the targeted application of residual stresses influenced by a controlled subsequent cooling offers great potential. The additional process parameter, i.e. temperature, compared to classical forming techniques increase the range of influence on e.g. deformation state and microstructure evolution. This contribution specifically analyses the relation of cooling a hot formed part and the resulting residual stress evolution inside the material. A cylindrical specimen with eccentric hole is considered, cf. [1], to ensure inhomogeneous stress states.

On the basis of detailed experimental and numerical investigations on the macroscale, cf. [2], suitable material characterizations are carried out concerning all occurring microstructural phases. Additionally, complex thermal, mechanical and metallurgical interactions have to be taken into account as well. Evoked by cooling, phase transformations on the atomistic scale occur, which depend on the cooling route and vary locally due to the polycrystalline nature of the material. Thereby, residual stresses arise, which influence the final macroscopic properties of the component. This multiscale view coincides with the definition of residual stresses based on the length scales, see [3].

In this contribution, a numerical model for the cooling of a macroscopic component is presented which takes into account phase transformation. The multiscale view motivates the utilization of a two-scale Finite Element model to describe these microscopic phenomena. Resulting residual stress distributions are discussed.

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Davoli, Elisa

Title: Two-well linearization for solid-solid phase transitions

Abstract:
In this talk, we consider nonlinearly elastic, frame-indifferent, and singularly perturbed two-well models for materials undergoing solid-solid phase transitions in any space dimensions, and we perform a simultaneous passage to sharp-interface and small-strain limits. Sequences of deformations with equibounded energies are decomposed via suitable Caccioppoli partitions into the sum of piecewise constant rigid movements and suitably rescaled displacements. These converge to limiting partitions, deformations, and displacements, respectively. Whereas limiting deformations are simple laminates whose gradients only attain two values, the limiting displacements belong to the class of special functions with bounded variation (SBV). By Γ-convergence we identify an effective limiting model given by the sum of a quadratic linearized elastic energy in terms of displacements along with two surface terms. The first one is proportional to the total length of interfaces created by jumps in the gradient of the limiting deformation. The second one is proportional to twice the total length of interfaces created by jumps in the limiting displacement, as well as by the boundaries of limiting partitions. A key tool of our analysis is a novel two-well rigidity estimate for a model with anisotropic second-order perturbation. This is joint work with Manuel Friedrich (Univ. Münster).

Dondl, Patrick

Title: Relaxation and Numerical Implementation for a Model of Nonlinear Strain-Gradient Single-Crystal Elastoplasticity

We will consider a non-convex model of single-crystal elasto-plasticity, where the non-convexity arises through the imposition of a hard "single-plane" side condition on the plastic deformation. This well-posed variational model arises as the relaxation of a more fundamental "single-slip" model in which at most one slip system can be activated at each spatial point. The relaxation procedure is motivated by the desire for efficient, oscillation-free simulation of single-crystal plasticity, but it is not immediately obvious how to implement the strict side-condition (that at most one slip-plane may be activated at each point) numerically. Our approach to this problem is to regularize the side-condition by introducing a large, but finite, cross-hardening penalty into the plastic energy. The regularized model is then amenable to implementation with standard finite-element methods, and, with the aid of div-curl arguments, one can show that it Gamma-converges to the single-plane model for large penalization.

Eidel, Bernhard

Title: The resolution error in image-based microstructure modeling and its embedding into the unified error framework of FE-HMM

Abstract: A cornerstone of computational solid mechanics in the context of digital transformation are pixelized images of microstructures obtained from advanced tomography techniques. In this talk we propose a novel concept of a unified error analysis for image-based microstructure representations in uniform resolution along with adaptively coarsened finite element discretizations.
The key novel aspect is to distinguish between an error due to finiteimage resolution and a standard discretization error. This decomposition of the micro error is consistently embedded into the unified error framework of the Finite Element Heterogeneous Multiscale Method FE-HMM and FE^2 [1].
In descriptive examples of two-phase microstructures we investigate the quantitative relation of the micro error parts, consider their spatial distributions and their impacts on the simulation results both on the microscale and the macroscale in the context of computational homogenization. Beyond the examples considered here the concept is a rational tool in the transformation of raw image data into microstructure information. It endows the digital twin of real microstructures with validated characteristics for reliable, predictive simulations.
This is joint work with A. Fischer and A. Gote.

[1] B. Eidel, A. Fischer, A. Gote: From image data towards microstructure information and Accuracy analysis at the digital core of materials, ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik, in press (2020), DOI: 10.1002/zamm.202000245.

Friedrich, Manuel

Emergence of rigid polycrystals from atomistic systems

We investigate the emergence of rigid polycrystalline structures from atomistic particle systems. The atomic interaction is governed by a suitably normalized pair interaction energy, where the `sticky disk' interaction potential models the atoms as hard spheres that interact when they are tangential. The discrete energy is frame invariant and no underlying reference lattice on the atomistic configurations is assumed. By means of Gamma-convergence, we characterize the asymptotic behavior of configurations with finite surface energy scaling in the infinite particle limit. The effective continuum theory is described in terms of a piecewise constant field delineating the local orientation and micro-translation of the configuration. The limiting energy is local and concentrated on the grain boundaries, i.e., on the boundaries of the zones where the underlying microscopic configuration has constant parameters. The corresponding surface energy density depends on the relative orientation of the two grains, their microscopic translation misfit, and the normal to the interface. Joint work with Leonard Kreutz (Münster) and Bernd Schmidt (Augsburg).

Garza, David Padilla

Title: Dimension reduction through Gamma convergence in thin elastic sheets with thermal strain, with consequences for the design of controllable sheets

Abstract: In this work, we analyze thin elastic sheets with a wide class of spatially varying prestrains. Using techniques from (Friesecke, G., James, R. D., & Müller, S. (2002). A theorem on geometric rigidity and the derivation of nonlinear plate theory from three-dimensional elasticity), we derive a rigorous Gamma-convergence result for the limiting energy. We borrow from geometric generalizations of the Friesecke-James-Müller theory, e.g. work by Bernd Schmidt and later by Marta Lewicka and collaborators, and generalize their results to a wider class of geometric strains and elastic laws. Our main result involves convex integration type techniques found in [Lewicka, M., & Pakzad, M. R. (2017). Convex integration for the Monge–Ampère equation in two dimensions]. Our ansatz for the upper bound is qualitatively different from that associated with any classical plate theory; it suggests that in a region where the limiting configuration is locally planar, the presence of prestrain could induce wrinkling (we are grateful to Marta Lewicka for suggesting the use of an ansatz involving wrinkling). Our results provide a systematic framework for modelling and analyzing the design of controllable sheets.

Ginster, Janusz

Titel: On the Motion of Curved Dislocations in Three Dimensions: Simplified Linearized Elasticity

Abstract: In this talk we discuss a simplified equilibrium problem for a curved dislocation line in a three-dimensional domain. As the core radius tends to zero, we derive an asymptotic expression to characterize the induced elastic energy. We then obtain the force on the dislocation line as the variation of this expression and identify the highest order terms explicitly. As a main ingredient, we present an explicit asymptotic formula for the induced elastic strain which depends on the curvature of the dislocation line and thus highlights the difference to existing work on straight dislocation lines. Eventually, we present results on the corresponding dynamics. The presented methods are a blueprint for the more physical setting of linearized isotropic elasticity.

This is joint work with I. Fonseca and S. Wojtowytsch.

Görthofer, Johannes

A modular and convex framework to compute anisotropic damage evolution

We present a modular framework for anisotropic damage evolution based on the full compliance tensor as the primary damage variable. Inspired by earlier work of Govindjee et al. [IJSS, 1995], we propose a small-strain generalized standard material model with a convex free energy. The dissipation potential may be assembled in a modular fashion based on stress-extraction tensors and damage-hardening functions, in analogy to yield surfaces in associative elastoplasticity. The resulting model precludes localization and permits replicating stable damaging processes in anisotropic media. Last but not least, we apply our model to predict damage evolution in a fiber-reinforced thermoset by designing damage-hardening functions and stress-extraction tensors based on Puck's anisotropic failure criteria.

Idiart, Martin Ignacio

Title of the talk: Model reduction by mean-field homogenization in viscoelastic composites

Abstract of the talk: A homogenization scheme for viscoelastic composites proposed by Lahellec and Suquet (2007, Int. J. Solids Struct. 44, 507) is revisited. The scheme relies upon an incremental variational formulation providing the inelastic strain field at a given time step in terms of the inelastic strain field from the previous time step, along with a judicious use of Legendre transforms to approximate the relevant functional by an alternative functional depending on the inelastic strain fields only through their first and second moments over each constituent phase. As a result, the approximation generates a reduced description of the microscopic state of the composite in terms of a finite set of internal variables that incorporates information on the intraphase fluctuations of the inelastic strain and that can be evaluated by mean-field homogenization techniques. In this work we provide an alternative derivation of the scheme, relying on the Cauchy-Schwarz inequality rather than the Legendre transform, and in so doing we expose the mathematical structure of the resulting approximation and generalize the exposition to fully anisotropic material systems. The scheme is then applied to random mixtures of a viscoelastic solid phase and a rigid phase. Results are reported for specimens subject to various complex deformation programs. The scheme is found to improve on earlier approximations of common use and even recover exact results under several cirumstances. However, it can also generate highly inaccurate predictions as a result of the loss of convexity of the free-energy density. An auspicious procedure to partially circumvent this issue is advanced.

Ortiz, Michael

Title: Plasticity with non-convex elastic-domain, symmetric div-quasiconvexity and stress-space relaxation

Abstract: It has been long known in geophysics, but not widely recognized in mechanics, that materials such as silica glass exhibit anomalous pressure-dependent strength characterized by a strongly non-convex elastic domain. This lack of convexity violates the standard Drucker principles of classical plasticity, including the principle of maximum dissipation, and may result in fine-scale patterning of the stress field. In order to understand these phenomena, we consider problems of static equilibrium in which the primary unknown is the stress field and the solution maximizes a complementary energy subject to equilibrium constraints. A necessary and sufficient condition for the sequential lower-semicontinuity of such functionals is symmetric div-quasiconvexity in the sense of Fonseca and Müller's A-quasiconvexity. We specifically consider the example of the static problem of plastic limit analysis and seek to characterize its relaxation in the non-standard case of a non-convex elastic domain. We show that the symmetric div-quasiconvex envelope of the elastic domain, which describes the effective or macroscopic plastic behavior of the material, can be characterized explicitly by means of a rank-2 hull construction for isotropic materials whose elastic domain depends on pressure and Mises effective shear stress. The resulting relaxed elastic domain closely matches that obtained by means of molecular dynamics calculations for silica glass. Remarkably, owing to the equilibrium constraint the relaxed elastic domain can still be strongly non-convex, which shows that, contrary to Drucker's postulates, convexity of the elastic domain is not a requirement for existence in plasticity.

Pastukhova, Svetlana

Svetlana Pastukhova "Error estimate in homogenization of fourth order elliptic operators"

ABSTRACT
In the whole space of arbitrary dimension, fourth order elliptic operators with periodic highly oscillating coefficients are considered. In the case of dimension two, such kind operators appear in elasticity theory on thin plates made of small period composites. Let epsilon be the linear size of the periodicity cell. The homogenized operator (or the limit operator, as epsilon, the parameter of nonhomogeneity, goes to zero) is of the same ellipticity class like the original operator, but with constant coefficients.
We prove that L^2-operator norm of the difference between the resolvents of the original and the homogenized operators is of order epsilon^2. This result sharpens the homogenization error esimate of order epsilon known earlier for the case under consideration.

Pelech, Petr

Title: "Separately Global Solutions to Rate-Independent Systems - Applications to Large-Strain Deformations of Damageable Solids"

Abstract: "Rate-independent systems (RIS) are characterized by the lack of any internal time length scale: rescaling the input of the system in time leads to the very same rescaling of its solution. In continuum mechanics, rate-independent models represent a reasonable approximation whenever the external conditions change slowly enough so that the system can always reach its equilibrium. This applies if inertial, viscous, and thermal effects can be neglected. RIS have proven to be useful in modeling of hysteresis, phase transitions in solids, elastoplasticity, damage, or fracture in small and large strain regimes.

The talk introduces the notion of separately global solutions for RIS with non-convex functionals and describes an existence result for a model of bulk damage at large strains. The analysis covers non-convex energies blowing up for extreme compression, yields solutions excluding interpenetration of matter, and allows for handling nonlinear couplings of the deformation and the internal variable, which emerges e.g. from the interplay between Eulerian and Lagrangian description. The result extends the theory developed so far in the small strain setting.

This is a joint work with Elisa Davoli (TU Wien) and Martin Kružík (ÚTIA CAS)."

Rohan, Eduard

"Homogenization of the vibro-acoustic transmission on perforated elastic plates with metamaterial properties"

ABSTRACT:
Based on our previous work, we propose a homogenized model of acoustic waves propagating through periodically perforated elastic plates with metamaterial properties. Such structures enable to suppress the acoustic transmission for selected frequency bands. We replace the fluid-structure interaction problem in a 3D complex geometry by effective transmission conditions prescribed on the acoustic metasurface associated with the plate mid-plane. The metamaterial properties of the elastic structure perforated by cylindrical holes are due to soft elastic inclusions serving for resonators. The interface conditions are derived by homogenization of the vibroacoustic fluid-structure interaction problem imposed in a transmission layer embedding the elastic plate described using the Reissner-Mindlin theory. Asymptotic analysis with respect to the layer thickness, proportional to the plate thickness and to the perforation period yields the Dirichlet-to-Neumann operator given in an implicit form. It involves a jump in the acoustic potential and its normal one-side derivatives across the interface which represents the plate with a given thickness. The homogenized model of the layer involves frequency-dependent effective parameters which change their signs, hence inducing a band-gap effect. An efficient method for computing these parameters is suggested. The global problem of the acoustic wave propagation in a waveguide fitted with the plate is solved using the finite element method. The homogenized interface allows for a significant reduction of the computational model. Numerical illustrations of the vibroacoustic transmission are presented.

Ruggeri, Michele

Title: Numerical approximation of the inertial Landau-Lifshitz-Gilbert equation

Abstract: We consider the numerical approximation of the inertial Landau-Lifshitz-Gilbert equation (iLLG), which describes the dynamics of the magnetization in ferromagnetic materials at subpicosecond time scales. We present two fully discrete numerical schemes, both implicit and based on first-order finite elements, which preserve the inherent unit-length constraint of iLLG at the vertices of the underlying mesh, and generate approximations that converge towards a weak solution of the problem.

Sarhil, Mohammad

Title: Aspects of a finite element formulation for the relaxed micromorphic model

Authors:
Mohammad Sarhil, Jörg Schröder, Lisa Scheunemann, Patrizio Neff

Abstract:
Metamaterials are artificially designed structures which can tailor material properties such that they obtain their properties not only from the base materials but mainly their specific engineered structures. Metamaterials emerged from the fields of electromagnetics and optics and expanded to mechanical, acoustic, and thermal properties. Their unconventional applications and properties such as frequency band gaps, negative refraction, filtering/focusing capabilities, and others are of great interest nowadays [1].

The exotic behavior of the mechanical metamaterials cannot be described by the classical Cauchy theories and generalized continuum theories are needed, such as Cosserat, second-gradient, or micromorphic theories [2-3]. Lately, the relaxed micromorphic model was introduced [3-4], which reduces the complexity of the general micromorphic model and successfully solves many problems in capturing the main microscopic and macroscopic mechanical characteristics of the targeted metamaterials (for example stiffness and anisotropy). It shows superior behavior compared to other micromorphic models for the asymptotic case when the characteristic length of the microstructure approaches infinity. The energy functional of the relaxed micromorphic model includes the Curl of a nonsymmetric micro-distortion field, similar to the Cosserat model, but keeps the full kinematics of the micromorphic theory and seeks the solution of the micro-distortion in H(Curl) space while the macroscopic displacement solution is in H^1 space.

In our presentation, we introduce a H(Curl) conforming finite element formulation for the relaxed micromorphic model and compare it with a classical non-conforming Lagrange finite element formulation. We show several numerical examples illustrating the differences of the solutions.

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Schäffner, Matthias

Title: Representative volume element approximations for laminated nonlinearly elastic random materials

Abstract: The representative volume element (RVE) method is a popular method for approximation of homogenized properties of random materials. In recent times, a significant progress has been made in understanding the approximation error for linear elliptic equations and convex integral functionals. In this context, we study nonlinearly elastic randomly laminated composite materials, and thus homogenization of a nonconvex integral functional. Under appropriate assumptions on the energy density (frame indifference; minimality non-degeneracy and smoothness at identity) and on the rapid decay of correlations of the random material, we establish an error estimate of order L-1/2 for the RVE approximation and its first two

derivatives in a neighborhood of the set of rotations. The presentation is based on a joint work with Stefan Neukamm and Mario Varga.

Schneider, Matti

Titel: Periodize the law? - A computational study of stochastic homogenization for particle-filled composites

Kurzzusammenfassung:
Digital volume images of composite microstructures naturally induce artifacts for particles which intersect the boundary of the domain. The effects of this boundary treatment are of interest, both, from an engineering and an analytical point of view.
We investigate the effects of intersecting boundary particles for two- and three-dimensional composites with spherical and cylindrical fillers at industrial volume fractions by computational studies. In this talk, the findings are reported.

Schubert, Richard

The influence of effective viscosity on particle sedimentation

Abstract: We discuss the rigorous derivation of mean-field limits for sedimenting particles. To leading order we obtain a coupled transport-Stokes equation. To next order in the volume fraction of the sedimenting particles the suspension obtains an effective viscosity expressed by Einstein's formula, which in turn has an effect on sedimentation which we are able to characterize. For both orders we provide quantitative approximation estimates in terms of the Wasserstein distances of the particle densities and L^p distances of the fluid velocities. The effective viscosity is due to very singular interactions of the particles. We are able to tame these by improving on previous results on mean-field limits. This is joint work with R. Hoefer.

Stefanelli, Ulisse

Title: Crystallization in a one-dimensional periodic landscape

Abstract: I will discuss the crystallization problem for a finite, one-dimensional collection of identical hard spheres in a periodic energy landscape. This corresponds to a simplified model for ionic dimers, as well as epitaxial growth on a crystalline substrate in presence of lattice mismatch. Depending on the commensurability of the radius of the sphere and the period of the landscape, different regimes arise. The emergence of arbitrarily long crystals is generically not to be expected. This is joint work with Manuel Friedrich.

Tribuzio, Antonio

Nucleation and growth of lattice crystals

Abstract: we use the minimizing-movements approach to study an evolution of spin-systems defined on the two-dimensional square lattice of amplitude depending on a vanishing parameter ε. The driven energy is given by a nearest-neighbours anti-ferromagnetic potential.
We analyze both the discrete and the continuous (limit, as ε goes to 0) flow from a geometric point of view identifying spin-systems with the union of lattice squares corresponding to the positive statuses of the system. Through this identification, the anti-ferromagnetic energy corresponds to a negative perimeter. We consider evolutions starting from a single point (nucleation).

We show that, the competition between short-range-repulsion (negative perimeter) and long-range-attraction (dissipation) produces a checkerboard pattern of the minimizers at the discrete level and a "backward" evolution at the continuous one. We prove that the scheme converges to a family of expanding

sets with constant velocity. The "shape" of the limit motion depends on the choice of the scale between the time and space parameters and on the norm defining the dissipation term.

Xu, Bai-Xiang

Title: Multiphysics phase-field modeling and simulation of microstructure evolution during additive manufacturing

Abstract: There exists large potential for the mechanical and functional property of the additively manufactured part to be optimized with respect to the process and material parameters. Compared with the expensive trial-and-error principle, physical models and numerical simulations are much more efficient in terms of both cost and time. They allow massive parameter studies which can provide large database for statistical analysis such as machine learning to extract the process-microstructure-property relation. One needs hence a reliable physical model, which can recapture the processing and the microstructure development. In this work we present a thermodynamically consistent nonisothermal phase-field model and the finite element simulations of microstructure evolution (pore and grain structure) during powder bed fusion additive manufacturing of metallic materials. We study both the selective sintering (SS) and selective melting (SM). The model includes simultaneously complex underlying physics, such as extreme heat diffusion, melting, solidification and grain coalescence. The models are parameterized using measured thermodynamic and kinetic data. For the process simulation, we overcome the numerical challenges on powder bed deposition, power injection and strategies to reduce the computation cost by a novel algorithm analogy to minimum coloring problem and grain tracking approach. Simulation results will be shown for e.g. stainless steel 316L and Fe-alloys. We reveal the influences of process parameters e.g. the laser power and scan speed on the microstructure features, such as porosity, surface morphology, geometric variation of grains and densification. The simulation results will be discussed in comparison with the experimental data available in the literature.