ANNUAL MEETING 2022 in Regensburg

Projekt 1:

Philipp Tscherner Freiburg

Modeling and Simulation of Paper Folding

In this project we study foldable objects by means of modeling, numerical simulation and geometrical analysis. For the latter, a relation between the fold angle, the geodesic and normal curvature of a folding arc is derived,
giving rise to interesting geometrical observations of structures involving curved folds. To model objects including kinks, a 2D energy is identified as the Γ-limit of a 3D elastic energy that accounts for disontinuities of the deformation gradient along a prescribed curve. The reduced model is discretized by a discontinuous Galerkin method that allows for a practical description of foldable structures by neglecting gradient jumps of the deformation along the folding curve. An error estimate is derived for the corresponding linear model that describes configurations with small deflections and does not include the isometry condition. The discretized nonlinear model, that is based on a reconstruction of the Hessian and a relaxation of the isometry condition, Γ-convergences to the continuous 2D model
under appropriate density assumptions on smooth folded isometries. Various numerical experiments are carried out to study the physical behaviour of foldable objects like flytraps.

Projekt 2:

Timo Neumeier Augsburg

Numerical Relaxation in Continuum Damage Mechanics

In this talk, we focus on the numerical relaxation of a pseudo time incremental model for continuum damage mechanics in the finite strain setting.
Therefore we discuss feasible algorithms for the approximation of semi convex hulls like the rank-one and the polyconvex envelope.
Due to the lack of convexity but the presence of weaker convexity notions, the relaxed model is able to capture strain-softening of the material while also providing mesh independent approximations.

Projekt 3:

Marius Harnisch Dortmund

On the data-driven simulation of inelastic material behavior using history surrogates

In this contribution, we present a novel approach to consider inelastic and path-dependent material behavior based on the data-driven mechanics, introduced in 2016 by Kirchdoerfer and Ortiz. The approach is based on a suitable 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. These quantities are used as substitutable modules that affect both data generation and data-driven simulation and thereby maintain the structure of the original framework, allowing for an extension of existing codes for elasticity in a straight-forward fashion.

Based on this, we show results of different inelastic processes, e.g. plasticity or phase transformations in shape memory alloys, and different non-monotonic loading paths.

Projekt 4:

Jonathan Fabiszisky Münster

Multiscale structures in compliance minimization

As a model problem for variational pattern formation in materials science we consider an optimal design problem, i.e. we aim to optimize the topology and geometry of an elastic material in a two-dimensional square domain. We minimize a weighted sum of the volume, compliance (the work done by the load) and perimeter of the material distribution under a prescribed boundary load. We are particularly interested in the asymptotic behaviour when the weight of the regularizing perimeter term tends to zero. While the optimal pattern for uniaxial and shear-type boundary loads is already partly understood, the case of a hydrostatic boundary load is completely open. As a candidate for a nearly optimal structure we combine known optimal structures for circular domains with a circle packing similar to a so-called Apollonian gasket. To show the optimality of this construction, we currently investigate ideas for lower bounds on the design cost.

Projekt 5:

Sergio Conti Bonn

Variational modeling of paperboard delamination under bending

Laminated paperboard consists of several sheets, which may separate under bending conditions. We develop a variational model and use it to discuss several regimes, with different degrees of delamination, which might occur under bending. The upper bounds for the energy are partially matched by scaling lower bounds. This is based on joint work with Patrick Dondl and Julia Orlik.

Projekt 6:

Alberto Maione / Hoa Le Freiburg

Part 1: Multi-material model and shape optimization for bending and torsion of inextensible rods

In this talk I present a model for the optimization of bending and torsional rigidity of non-homogeneous elastic rods, by studying a sharp interface shape optimization problem with perimeter penalization, that treats the torsional and bending rigidity as objectives. Once incorporated a diffuse interface approach, we show that, as a consequence of a Γ-convergence result, the sequence of minimizers of the diffuse interface approach convergences to the minimizer of the sharp interface problem, as the thickness of the interface tends to zero.

In the last part of the talk, I will show a numerical approximation of solutions to the phase field problem using a steepest descent approach and connected the results to the development of plant stems morphology.

This is a joint work with Patrick Dondl and Steve Wolff-Vorbeck (University of Freiburg).

Part 2: Atomistic simulation of Dislocation roughness in High-entropy alloys

In complex concentrated alloys, dislocations roughen at finite temperatures due to thermal fluctuations and local chemical distortion. Analyzing roughness profiles of dislocation lines at finite temperatures can provide insight into their line tension and depinning stress. Here, we use large-scale molecular dynamics simulations to study the dislocation fluctuation of a Fe-Ni-Cr-Co-Cu equicomposition High-entropy alloy and compare with its corresponding average alloy.

The thermal effects and chemical fluctuations will then show up in measures of the power-spectral density of displacements (PSD) and displacement-difference autocorrelation function (ACF) of dislocation roughness. Results indicate that PSD and ACF are separated into long-wavelength and short-wavelength regimes, where solute concentration and thermal effects are dominant, respectively. Both regimes exhibit power-law scaling. The High-entropy alloy and its average alloy show a good agreement in the short-wavelength regime, where the spectrum reflects the line tension.

Projekt 7:

Florian Behr Regensburg Ghina Jezdan Bochum

Analytical and numerical study of energies in pressure dependent plasticity.

Experiments conducted in granular media like clay, silt, or sand show complex structures which cannot be explained as simple shear bands. Materials in this class are usually heterogeneous mixtures of fluids, usually air and water, and particles that have little to no cementation. The shear strength is provided by friction and interlocking of the particles. This generally leads to pressure dependent plastic behavior.

Consequently, models in soil mechanics require pressure-dependent yield surfaces resulting, in contrast to models in crystal plasticity, in non-associated flow rules, which have not been studied as extensively as associated ones. In this study, we introduce a model capable of explaining the occurrence of the complex structures mentioned above starting from a time-incremental variational formulation.

We consider a basic model giving a reduced description for plasticity in soil mechanics with as few parameters as possible while retaining the essential features of the full model. The goal is to capture the complexity seen in experiments by considering the stability properties of the emerging microstructures. As expected, these complex structures lead to challenging questions concerning numerical simulations, which can be resolved employing a relaxed model in the implementation.

Projekt 9:

Bai-Xiang Xu Darmstadt Herbert Egger Linz

Variational quantitative phase-field modeling of non-isothermal sintering process during additive manufacturing

Phase-field modeling has become a powerful tool in describing the complex pore-structure evolution and the intricate multi-physics in non-isothermal sintering processes. However, the quantitativeness of conventional variational phase-field models involving diffusive processes is a challenge. Artificial interface effects, like the trapping effects, may originate at the interface when the kinetic properties of two opposing phases are different. On the other hand, models with prescribed antitrapping terms do not necessarily guarantee the thermodynamic consistency of the model. Thus variational quantitative phase-field models are desired.

Though such models exist for solidification, there is no related work addressing the interfaces in non-isothermal sintering, where the free surfaces between the solid phase and surrounding pore regions exhibit strong asymmetry of mass and thermal properties. Additional challenges arise due to the conserved order parameter describing the free surfaces. In this work, we present for the first time a variational and quantitative phase-field model for non-isothermal sintering processes with a coupled Allen-Cahn and Cahn-Hilliard equations. The model is derived via an extended non-diagonal model with no restriction on the range of diffusivity ratio. The model evolution equations naturally have cross-coupling terms between the conserved kinetics (e.g. mass and thermal transfer) and the non-conserved ones (e.g. grain growth). Via asymptotic analysis, these terms are shown to be instrumental in ensuring the elimination of interface effects. Moreover, we demonstrate that the trapping effects and existence of surface diffusion in conservation laws are direction-dependent. An anisotropic interpolation scheme of the kinetic mobilities which differentiates the normal and the tangential directions along the interface is discussed. Numerically, we demonstrate the importance of the cross-couplings and the anisotropic interpolation.

The underlying energy/entropy– dissipation or gradient flow structure of the derived models is of great importance, both, for the analysis and the systematic numerical approximation. Structure preserving discretization schemes for coupled Allen-Cahn, Cahn-Hilliard, and non-isothermal phase-field models are examined. The correct handling of cross-diffusion terms, thermodynamic consistency, as well as well- posedness of the models is studied on the continuous and discrete level.

Projekt 10:

Vanessa Hüsken **Duisburg**

Very singular solutions of a nonlinear Cosserat elasticity model for solids

For a geometrically non-linear Cosserat elasticity model for solids, we explore how big the singular set of a critical point for the corresponding Cosserat energy functional can get. During last year's annual meeting, we presented a technique to construct (fixed) dipole pairs of singularities. This method is put to use, as we construct smooth boundary data in such a way that any restricted energy minimizer subject to those boundary data must have at least N singular points, where N is an arbitrary given number.

Projekt 11:

Martin Heida **Berlin**

Elasticity on randomly perforated domains

Abstract: We study homogenization of elasticity on randomly perforated domains with globally unbounded Lipschitz constant. We will see that already in the case of linear elasticity, homogenization takes place in L^p with p strictly smaller than 2.

Projekt 12:

Friederike Röver / Stefan Prüger Freiberg

Co-Design of Variationally-Consistent Formulations of Chemo-Mechanics and a Parallel Solver Framework

Variational formulations of coupled multi-field boundary value problems give a clear understanding of the mathematical structure of the problem. This can be used for efficient solution strategies in the form of tailored solvers. The focus of this talk is on the results obtained for the co-design of the theoretical model and parallel solvers. We consider the variational framework of a chemo-mechanical boundary value problem, outlined in [L. Boeger, et al., Int. J. Solids Struct., 121, pp. 257–274,2017], which incorporates a full coupling of mechanics and diffusion in a finite deformation setting. From rate type potentials, we can either derive a minimization or a saddle point formulation. As a parallel solver, we consider, in particular, the FROSch framework [A. Heinlein et al., In: Domain Decomposition Methods in Science and Engineering XXV, pp. 176–184, Springer, 2020] of the Trilinos software library, which contains a parallel implementation of the GDSW overlapping Schwarz domain decomposition preconditioner with an energy minimizing coarse space. The crucial advantage of the GDSW precondioner is that it allows an algebraic construction from the fully assembled stiffness matrix. We present results of a first study, where we consider the fully algebraic application of the preconditioner to the fully coupled problem outlined above. We used the deal.II software library [D. Arndt, et al, J. Numer. Math., 28(3), pp. 131–146, 2020] for the finite element implementation of the weak formulation and made use of the interface to the parallel linear algebra infrastructure of Trilinos to construct the FROSch preconditioner.

Projekt 13:

Samira Boddin / Felix Rörentrop

Simulation and Analysis of phase-field damage models for brutal crack Evolution

The modelling of cracks has been an intensely researched topic for decades – both from the mechanical as well as from the mathematics point of view. As far as the modelling of sharp cracks/interfaces is concerned, the resulting free boundary problem is numerically very challenging.
For this reason, diffuse approximations in the sense of phase-field theories have become very popular, cf. [1]. Within this talk, the focus is on rate-independent damage models. In this case, the resulting phase-field approximation is characterized by (incrementally defined) non-convex optimization problems. This non-convexity, in turn, gives rise to a discontinuous evolution of crack propagation (so-called brutal crack growth) and therefore, solution concepts have to be carefully chosen and designed. One sound concept is that proposed by Efendiev & Mielke, cf. [2]. Within this talk, the framework [2]

is implemented into the Finite-Element-Method and carefully analysed from a physics and mathematical point of view. Particularly, the effect of different norms in the framework [2] is investigated.

[1] B. Bourdin, G.A. Francfort, J-J. Marigo, Numerical experiments in revisited brittle fracture, Journal of the Mechanics and Physics of Solids 48(2000), 797-826
[2] M. A. Efendiev, A. Mielke, On the Rate-Independent Limit of Systems with Dry Friction and Small Viscosity, Journal of Convex Analysis 13(1), 151-167

Projekt 14:

Matthias Liero **Berlin**

Viscoelastodynamics of solids at large strains coupled to diffusion processes
Vortragender: Matthias Liero

We discuss a model describing the coupling of diffusion processes and the viscoelastic deformation of a porous solid at large strains.
The equations are formulated in the reference configuration by using the concept of second-grade nonsimple materials. The existence of weak solutions
in the quasistatic setting, that is inertial forces are ignored, via time discretization is discussed.

Projekt 15:

Mohammad Sarhil **Essen**

Modeling the size-effects of metamaterial beams under pure bending via the relaxed micromorphic model

Metamaterials are artificial structures that exhibit the size-effect phenomena which can not be captured by the standard Cauchy elasticity or first-order homogenization methods. Generalized continuum theories can be suitable tools for the description of such materials. In our work, we adopt the relaxed micromorphic model which has been used successfully to model the main microscopic and macroscopic mechanical properties of the assumed metamaterials for many applications [1-2]. It uses fewer material parameters compared to the classical micromorphic theory and exhibits a bounded stiffness for the small specimen. The relaxed micromorphic model employs the Curl of a micro-distortion field, similar to the Cosserat model, and therefore tangential conforming finite elements are needed [3].

In our presentation, we investigate the size-effects of metamaterial beams under pure bending. Reference solutions of metamaterial beams with fully discretized microstructures are constructed for different loading cases. The homogenous relaxed micromorphic model is used then to model these beams. The identification of the material parameters, the anisotropy properties, the boundary conditions and other aspects will be discussed.

REFERENCES
[1] P. Neff, I.D. Ghiba, A. Madeo, L. Placidi, G. Rosi. A unifying perspective: the relaxed linear micromorphic continuum. Continuum Mech. Thermodyn. 26, 639–681 (2014).
[2] P. Neff, B. Eidel, M.V. d'Agostino, M. Madeo. Identification of scale-independent material parameters in the relaxed micromorphic model through model-adapted first order homogenization. J. Elast. 139, 269–298 (2020).[3] J. Schröder, M. Sarhil, L. Scheunemann, P. Neff.

Lagrange and H(curl,B) based Finite Element formulations for the relaxed micromorphic model (to appear in Comput. Mech.)

Projekt 16:

Antonio Tribuzio Heidelberg

Scaling laws for multi-well nucleation problems

Abstract: In this talk, we study scaling laws for nulceation problems which are motivated by models for shape-memory alloys.
More precisely, we discuss optimal energy scaling of inclusions of a phase with several variants (martensite) inside a parent phase (austenite), for various model problems in two and three dimensions.
The energy term is given by a singularly-perturbed multi-well elastic energy (without gauge invariances).
We provide scaling results in the volume and the singular perturbation parameter for settings in which the surrounding parent phase is in the first-, the second- and the third-order lamination-convex hull of the wells of the "martensite phase".
Furthermore, we provide a corresponding result for the setting of an infinite-order laminate which arises in the context of the Tartar square.

Projekt 17:

Jiri Zeman Augsburg

Continuum models for elastic and brittle nanowires derived from an atomistic description by Gamma-convergence

Starting from a particle system with short-range interactions, we derive continuum models for the bending, torsion or brittle fracture of inextensible rods moving in three-dimensional space. In our derivation we study limits of the rod thickness and interatomic distance simultaneously tending to zero. If the two quantities are of the same order of magnitude, this leads to a novel theory for ultrathin rods composed of finitely many atomic fibres, which incorporates surface energy and new discrete terms in the limiting functional. Further, in the elastic-brittle case, fracture energy in the Gamma-limit is expressed by an implicit cell formula, which covers different modes of fracture, including (complete) cracks, folds and torsional cracks. In special cases, the cell formula can be significantly simplified. Our approach applies e.g. to atomistic systems with Lennard-Jones-type potentials and is motivated by the research of ceramic nanowires.

Projekt 18:

Jonas Lendvai Karlsruhe

On the influence of different boundary conditions when computing the effective crack energy of random heterogeneous materials

-Recent stochastic homogenization results [1] confirmed the existence of representative volume elements (RVEs) for the Francfort-Marigo model of brittle fracture [2] under anti-plane shear loading [3,4]. The including multicell formula relies on initial notches which may be interpreted as Dirichlet boundary conditions. For other physical problems, e.g., thermal conductivity or linear elasticity, the imposed boundary conditions play less and less of a role for increasing volume-element size. However, the practical size of the RVEs may be strongly influenced by the kind of boundary conditions.

To study different boundary conditions, we introduce a strategy for computing the effective crack energy in the 2D case with the help of fast marching algorithms [5]. Based on these techniques, we study the influence of the boundary conditions on the effective crack energy.

[1] F. Cagnetti, G. Dal Maso, L. Scardia, and C. I. Zeppieri, Arch. Rational Mech. Anal., (233), 935–974, 2019.
[2] G. A. Francfort and J.-J. Marigo, J. Mech. Phys. Solids, (46), 1319–1342, 1998.
[3] M. Schneider, Int. J. Numer. Methods. Eng., (121), 1367–1387, 2020.
[4] F. Ernesti and M. Schneider, Int. J. Numer. Methods. Eng., (122), 6283–6307, 2021.
[5] J. Sethian, PNAS, (93), 1591–1595, 1996.

Projekt 19:

Marita Thomas **Berlin**

First-order formulation for dynamic phase-field fracture in visco-elastic materials

We investigate a model for dynamic fracture in viscoelastic materials at small strains. The sharp crack interface is regularized with a phase-field approximation, and for the phase-field variable a viscous evolution with a quadratic dissipation potential is employed. A non-smooth penalization prevents material healing. The viscoelastic momentum balance is formulated as a first order system and coupled in a nonlinear way to the non-smooth evolution equation of the phase-field. We give a full discretization in time and space, using a discontinuous Galerkin method for the first order system. Based on this, we show the existence of discrete solutions and, as the step size in space and time tends to zero, we discuss their convergence to a suitable notion of weak solution of the system. Simulation results are presented and future research directions are addressed.
This is joint work with Sven Tornquist (WIAS), Christian Wieners (Karlsruhe), and Kerstin Weinberg (Siegen).