Abstracts GAMM Microstructures (Freitag, 28. Januar 2022)

1. Nicolas Clozeau (Wien):

Title: BIAS IN THE REPRESENTATIVE VOLUME ELEMENT METHOD: PERIODIZE THE ENSEMBLE INSTEAD OF ITS REALIZATIONS

We consider a model problem of diffusion or conductivity in a random medium (for instance, an heterogeneous domain obtained by mixing randomly two different phases, one being the matrix and the other the inclusions). The model that we use takes the form of an uniformly elliptic equation with high oscillatory (at scale S<<1) and random coefficient. The goal of this work is to analyse the approximation of the homogenized coefficient by the representative volume element method, that is when we replace the whole space by a large torus of size L. This operation makes the corrector equation easy to solve numerically and provides a natural approximation of the homogenized coefficient by the one coming from the periodic homogenization theory. In the analysis of the error, the variance suffers from two types of error: a random random (that is the fluctuation around its expectation) and a systematic error (that is the difference between the homogenized coefficient and the expectation of the approximation). We focus in this work on the systematic error and we characterize its asymptotic behaviour as L goes to infinity. We show that, in the particular case where the law is generated by a stationary Gaussian field, the asymptotic of the systematic error is characterized by a deterministic matrix depending on the first and second-order correctors, the gradient of the covariance function and a fourth-order tensor involving the whole space Green’s function of the homogenized elliptic operator.

2. Thorsten Bartel (TU Dortmund):

Title: Energy relaxation methods and its relation to modern data-based schemes

Energy relaxation methods have been successfully implemented in material models and for algorithms simulating inelastic material behavior in recent years. This includes phenomena such as plasticity and martensitic phase transformations. Current enhancements also consider coupled material behavior, such as in magnetic shape memory alloys. The advantage of this methodology is its direct relation to proofs of existence and uniqueness of solutions. Moreover, it offers a remarkable correlation between the hypothetical microstructures in the models (e.g. laminates) and the real existing ones. Thus, there is also a physical motivation and interpretation of these approaches in addition to the well-motivated mathematical foundation.
Currently, more and more data-based methods and algorithms are being established with the aim of simulating the behavior of specific materials. Basically, these methods serve as a replacement for conventional material models. It is often assumed that the required data sets for these methods can be determined from experiments alone, and that the real material behavior is thus very accurately represented. However, this should be viewed critically, since

it is still challenging to capture the spatially multidimensional material behavior at all or well enough through experimental data.
We therefore approach this topic rather with the argument that material models should serve as the basis for the data sets. Especially with the above mentioned energy relaxation methods, data sets can be generated which contain or represent all advantages of this theory.
Furthermore, with the extension of the data-driven mechanics established by Kirchdoerfer and Ortiz in terms of inelastic material behavior, it is possible to use a computational scheme in which equilibrium and compatibility conditions are explicitly considered and fulfilled.
In this contribution, the above-mentioned aspects of material modeling and their implementation in the data-driven mechanics are addressed and supported by numerical examples.

3. Marco Bresciani (TU Wien):

Title: A reduced model for plates arising as low energy Γ-limit in nonlinear magnetoelasticity

We investigate the problem of dimension reduction for plates in nonlinear magnetoelasticity. The model features a mixed Eulerian-Lagrangian formulation, as magnetizations are defined on the deformed set in the actual space. We consider low-energy configurations by rescaling the elastic energy according to the linearized von Kármán regime. First, we identify a reduced model by computing the Γ-limit of the magnetoelastic energy, as the thickness of the plate goes to zero. Then, we introduce applied loads given by mechanical forces and external magnetic fields and we prove that, under clamped boundary conditions, sequences of almost minimizers of the total energy converge to minimizers of the corresponding energy in the reduced model. Finally, we study quasistatic evolutions driven by time-dependent applied loads and a rate-independent dissipation, and we provide a further justification of the reduced model in the spirit of evolutionary Γ-convergence.

4. David Wiedemann (Universität Augsburg):

Title: Homogenisation of the Stokes equations on an evolving domain

We consider the homogenisation of the Stokes problem in a time-evolving porous medium. The evolution displaces fluid, which leads to a non-homogeneous Dirichlet boundary condition at the interface of the pore space with the solid matrix. In order to pass rigorously to the homogenisation limit, we transform the Stokes equations to a periodic substitute domain. The homogenisation result is a Darcy law with time- and space- dependent permeability tensor incorporating an additional source term for the pressure, which arises due to the local change of the porosity.

5. Viktor Shcherbakov (Universität Kassel):

Title: An adaptive time-discretization scheme for rate-independent systems

In the last two decades, several distinct solution concepts for rate-independent evolutionary systems driven by nonconvex energies have been suggested in an attempt to model properly jump discontinuities in time. Under these circumstances, numerical discretization schemes are needed that efficiently and reliably approximate directly that type of solution that one is interested in.
In this talk, we focus on a novel adaptive time-discretization scheme that is inspired by and based on the local minimization approach of Efendiev and Mielke (2006).
We employ a Moreau-Yosida regularization to approximate inequality Constraints enforcing the local minimality. In an abstract infinite-dimensional setting, we prove the convergence of time-discrete solutions to functions that are parametrized balanced viscosity solutions of the time-continuous problem provided that the discretization and regularization parameters are chosen appropriately. We test our scheme on a one-dimensional example and find a notable improvement compared with the original version.
This is a joint work with Dorothee Knees (University of Kassel).

6. Michele Ruggeri (TU Wien)

Title: Convergent finite element methods for antiferromagnets

Antiferromagnets (AFMs), magnetic materials in which neighboring magnetic moments tend to align antiparallel to each other, have been known for many years.
However, they have recently gained renewed interest, because several theoretical and experimental studies have shown that AFMs have feature that could lead to strong improvements of the functionality of spintronics devices.
In this talk, we discuss the numerical analysis of continuum models for AFMs.
We discuss two models: In the first one, the magnetic state of the AFM is described in terms of two unit-length vector fields representing the magnetization of two interacting sublattices. In the second one, the order parameter describing the material is one single unit-length vector field, the so-called Néel vector.
For both approaches, which in the dynamic setting require the solution of a suitable variant of the Landau-Lifshitz-Gilbert equation, we propose structure-preserving finite element methods and discuss their convergence.
This is joint work together with Stavros Komineas (University of Crete).

7. Martin Heida (WIAS Berlin)

Title: Upscaling of Intercalation electrodes featuring Cahn--Hilliard to Allen--Cahn transitions

We use two-scale convergence methods to study mathematical upscaling of a porous intercalation model with phase separation in the anode modeled by the Cahn--Hilliard equation. Depending on the topological connectedness of the anode and on the scaling of the mobility, we observe the transition of the Cahn--Hilliard equation to an Allen--Cahn equation or to a simple ODE during the upscaling process.

8. Alice Marveggio (TU Wien)

Title: Rates of convergence of the vector-valued Allen-Cahn equation towards multiphase mean curvature flow

The vector-valued Allen-Cahn equation with a multi-well potential is expected to approximate multiphase mean curvature flow in the limit of vanishing interface thickness. However, to the best of our knowledge, proving an unconditional convergence result for such a diffuse interface approximation for multiphase mean curvature flow has remained an open problem.
We present a proof for rates of convergence of the vector-valued Allen-Cahn equation towards multiphase mean curvature flow in the planar case d=2, assuming that a classical (smooth) solution to the latter exists. The result is valid for suitable multi-well potentials and starting from well-prepared initial data.
Our approach is based on a relative entropy technique inspired by [2] and, in particular, on the notion of gradient-flow calibration introduced in [1].
Beyond the planar setting, our results also apply to three-dimensional double bubbles (or more generally to evolving interfaces without quadruple junctions), relying on the existence of the gradient-flow calibration shown in [3].

[1] J. Fischer, S. Hensel, T. Laux, T. Simon. The local structure of the energy landscape in multiphase mean curvature flow: Weak-strong uniqueness and stability of evolutions. Preprint, 2020.

[2] J. Fischer, T. Laux, T. Simon. Convergence rates of the Allen-Cahn equation to mean curvature flow: A short proof based on relative entropies. SIAM J. Math. Anal., 52(6):6222–6233, 2020.

[3] S. Hensel and T. Laux. Weak-strong uniqueness for the mean curvature flow of double bubbles. Preprint, 2021.

9. Konstantinos Zemas (Universität Münster)

Title: " Geometric rigidity in variable domains and derivation of linearized models for elastic materials with free surfaces"

Quantitative rigidity results, besides from their inherent geometric interest, have played a prominent role in the mathematical study of models related to elasticity\plasticity. For instance, the celebrated rigidity estimate of Friesecke, James, and Müller has been widely used in problems related to linearization, discrete-to-continuum or dimension-reduction issues for functionals within the framework on nonlinear elasticity.

In this talk, I will present a generalization (in the physically relevant dimensions d=2,3) of this result to the setting of variable domains, where the geometry of the domain comes into play, in terms of a suitable integral curvature functional of its boundary. The estimate can be used to establish compactness in the space of generalized special functions of bounded deformation for sequences of displacements related to deformations with uniformly bounded elastic energy.

As an application, we rigorously derive linearized models for nonlinearly elastic materials with free surfaces by means of Gamma-convergence. In particular, we study energies related to epitaxially strained crystalline films and to the formation of material voids inside elastically stressed solids. This is joint work with Manuel Friedrich and Leonard Kreutz.

10. Claudia Raithel (TU Wien)

Title: Stochastic homogenization on domains with corners

In this talk we are concerned with the homogenization of linear elliptic PDEs in domains with corners, beginning with the simple situation of an angular sector in 2 dimensions. As opposed to the whole-space setting, on such a sector there exist non-smooth harmonic functions with homogeneous Dirichlet boundary data (depending on the angle of the sector). Our first main result is the construction of extended homogenization correctors corresponding to these harmonic functions and, furthermore, quasi-optimal (optimal up to a logarithmic factor) growth estimates for these ``corner correctors". For our construction it is necessary to first develop a large-scale regularity theory for a-harmonic functions in the sector, which implies a Liouville principle. Using our bounds for the corner correctors, we are then able to obtain a quasi-optimal error estimate for a new non-standard two-scale expansion that is adapted to the sectoral domain. This talk is based on joint work with Marc Josien and Mathias Schäffner.

11. Roman Indergand (ETH Zürich)

Title: The Effect of Thermal Fluctuations on the Ferroelectric Microstructure

Roman Indergand[1], Dennis M. Kochmann[2]
(Department of Mechanical and Process Engineering, Mechanics & Materials, ETH Zürich, 8092 Zürich, Switzerland, [1] iroman@mavt.ethz.ch, [2] dmk@ethz.ch.)

A phase-field (diffuse-interface) description of ferroelectricity and its numerical implementation via FFT-based spectral homogenization [1] is extended to account for the effects of finite temperature. This is achieved through a new constitutive model using statistical mechanics [2] to consider thermal lattice vibrations as well as by modifying the underlying

Ginzburg-Landau potential to depend on temperature. We observe that atomic-level thermal vibrations promote nucleation of needle-like domains at weak spots such as grain boundaries, which leads to a faster polarization reversal for subcoercive conditions and a more realistic ferroelectric microstructure.

We will discuss the development, implementation, and application of the temperature-aware phase-field model on the domain pattern evolution in ferroelectric ceramics [2] and on domain wall-pore interactions [3] in bulk lead zirconate titanate (PZT), which we demonstrate to admit better model predictions and comparison with experiments than comparable existing models.

REFERENCES

Vidyasagar, A., Tan,W., Kochmann, D. Predicting the effective response of bulk polycrystalline ferroelectric ceramics via improved spectral phase field methods. *Journal of the Mechanics and Physics of Solids,* Vol. 106, pp. 133 – 151, 2017.

Indergand, R., Vidyasagar, A., Nadkarni, N. , Kochmann, D. A phase-field approach to studying the temperature-dependent ferroelectric response of bulk polycrystalline PZT, *Journal of the Mechanics and Physics of Solids,* Vol. 144, 2020.

Indergand, R. and Kochmann, D. M., Effect of temperature on domain wall– pore interactions in lead zirconate titanate: A phase-field study. *Applied Physics Letters*, Vol. 119, 2021.

12. David Wiedemann (Universität Augsburg)

Title: Homogenisation of the Stokes equations on an evolving domain

We consider the homogenisation of the Stokes problem in a time-evolving porous medium. The evolution displaces fluid, which leads to a non-homogeneous Dirichlet boundary condition at the interface of the pore space with the solid matrix. In order to pass rigorously to the homogenisation limit, we transform the Stokes equations to a periodic substitute domain. The homogenisation result is a Darcy law with time- and space- dependent permeability tensor incorporating an additional source term for the pressure, which arises due to the local change of the porosity.

13. Peter Bella (TU Dortmund)

Title:Transition from wrinkles to flat state - Gamma convergence and beyond

I will discuss minimization of a non-convex singularly perturbed variational problem, which models transition region between wrinkled and flat state of a thin elastic sheet. Building on the previous result about optimal prefactor in the energy scaling law, we identify the Gamma-limit of the functional. This is a joint work with Alaa Elshorbagy.

14. Ameya Rege (DLR)

Title: On the impact of aggregation mechanism in modelling fractal materials

Ameya Rege*, Prakul Pandit, and Barbara Milow
Institute of Materials Research, German Aerospace Center, Cologne, Germany

In this contribution, the diffusive and ballistic nature of aggregate-formation in colloidal-like materials will be discussed. To this end, diffusion-limited and reaction-limited algorithms together with their cluster-cluster aggregation extensions will be considered. While the aggregating particles in such algorithms follow natural Brownian motion, an additional algorithm accounting for the linear motion of particles will also be analysed. The effect of these algorithms on the final network's structural and fractal properties will be presented. Furthermore, the application of the diffusion-limited cluster-cluster aggregation approach to model the sol-gel process in synthesising silica aerogels will be illustrated. The use of the finite element method in describing the mechanical properties of the generated model silica aerogels will be elucidated at the end [1].

References

1. Abdusalamov, R., Scherdel, C., Itskov, M., Milow, B., Reichenauer, G., & Rege, A. (2021). Modeling and Simulation of the Aggregation and the Structural and Mechanical Properties of Silica Aerogels. The Journal of Physical Chemistry B 125, 1944-1950.

15. Shivangi Aney (DLR)

Title: What is the influence of pore sizes on the macroscopic mechanical properties of open-porous cellular materials?

Shivangi Aney*, Barbara Milow, Ameya Rege
Institute of Materials Research, German Aerospace Center, Cologne, Germany

The influence of relative density on the macroscopic mechanical properties of open-porous cellular materials is well known within the scientific community [1,2]. However, for those materials that exhibit a rather wide range of the pore-size distributions over the length scale, it is still an open question as to whether the pore sizes influence the bulk properties of the solids. Within a numerical framework, the importance of considering these, along with the strut thickness and relative density was highlighted [3]. In this contribution, we have investigated computationally the effect of the three morphological parameters *viz*. the relative density, the pore-size distribution, and the pore-wall thickness on the mechanical properties of such open-porous materials. The results obtained demonstrate that while the relative density dictates the mechanical properties of open-porous solids, the effects of pore-sizes, pore-size distributions and pore-wall thickness are not negligible. These effects must be considered, particularly while developing materials showing a poly-disperse porous structure and requiring load-bearing capabilities under finite strains. As an example, the three-dimensional (3-d) porous network of cellulose aerogels is computationally reconstructed and the macroscopic material properties are described and validated against experimental data.

References

1. Gibson, L. J., Ashby, M. F., Schajer, G. S., & Robertson, C. I. (1982). The mechanics of two-dimensional cellular materials. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences* **382**, 25-42.

2. Gibson, I. J., & Ashby, M. F. (1982). The mechanics of three-dimensional cellular materials. *Proceedings of the Royal Society of London. A. Mathematical and Physical Sciences* **382**, 43-59.
3. Rege, A., Aney, S., & Milow, B. (2021). Influence of pore-size distributions and pore-wall mechanics on the mechanical behavior of cellular solids like aerogels. *Physical Review E* **103**, 043001