TECHNISCHE UNIVERSITÄT DRESDEN

DRESDEN concept

Mathematics of Continuum Mechanics

2nd Berlin Dresden Prague Würzburg Workshop

Technische Universität Dresden
Department of Mathematics
5 December, 2016

Berlin

Dresden

Würzburg

Prague

[1] Webpage: `https://tu-dresden.de/mn/math/wir/neukamm/die-professur/workshops//BDPW2`

1 General Information

Objectives

This workshop is the first of a series of "Berlin-Dresden-Prague-Würzburg"-meetings, which we plan to organize on a regular basis. The goal of these workshops is to bring together researchers (in particular young scientists) from the above mentioned regions interested in the Mathematics of Continuum Mechanics, ranging from analysis, modeling and simulation of materials, multiscale and evolution problems.

Organizers

Martin Kružík (Czech Academy of Sciences, Prague), Alexander Mielke (WIAS Berlin), Stefan Neukamm (TU Dresden) and Anja Schlömerkemper (U of Würzburg).

Location of the Lectures

The workshop will be hosted at TU Dresden. All lectures take place at

> Departement of Mathematics
> Willers-Bau (Zellescher Weg 12 - 14)
> **Room C207**
>
> `https://navigator.tu-dresden.de/etplan/wil/01/raum/219401.0220`

Dinner

The social dinner (no-host) takes place at "Brauhaus Watzke am Goldenen Reiter". It is located at Hauptstraße 1, see `https://goo.gl/maps/QVnDJ4vccv62`, next to the tram-station "Neustädter Markt" (Line 8,4,9) and in walking distance (< 10 minutes) to the train station "Dresden-Neustadt" (where almost all national trains depart).

Support

The organizers gratefully acknowledge financial support by the DFG in the context of TU Dresden's Institutional Strategy *"The Synergetic University"*.

Contact

Prof. Dr. Stefan Neukamm

email: stefan.neukamm@tu-dresden.de, phone: +49 351 463-34266

Visiting address:
TU Dresden, Department of Mathematics, Institute of Scientific Computing
Willersbau, room B208
Zellescher Weg 12-14
01069 Dresden

2 Program

10:30 – 11:25		**registration & welcome coffee**
11:25 – 11:30		**opening remarks**
11:30 – 12:20	Matthias Liero (WIAS Berlin)	On electrothermal feedback in organic light-emitting diodes
12:20 – 12:50		**poster blitz**
12:50 – 14:20		**lunch (buffet) and poster exhibition**
14:20 – 15:10	Petr Šittner (ASCR Prague)	Localized deformation in tensioned superelastic NiTi wire by 3D-XRD method
15:10 – 15:50		**coffee and poster exhibition**
15:50 – 16:40	Daniel Wachsmuth (Universität Würzburg)	Optimal control of a rate-independent evolution equation via viscous regularization
16:40		**closing**
ca. 18:00		*social dinner (no-host) at Brauhaus Watzke am Goldenen Reiter*

3 Posters

- Barbora Benešová (*Institute for Mathematics, University of Würzburg)*
  Incommensurateness in nanotwinning models of modulated martensites
- Jan Domurath *(Leibniz-Institut für Polymerforschung Dresden)*
  Viscosity amplification in dilute suspensions of non-spherical particles in a Carreau matrix fluid
- Andreas Fischle *(Department of Mathematics, TU Dresden)*
  Explicit Analysis of Optimal Cosserat Rotations
- Franziska Flegel *(WIAS Berlin)*
  Spectral localization vs. homogenization in the random conductance model
- Thomas Frenzel *(WIAS Berlin)*
  EDP-convergence for delamination and a wiggly energy model
- Hanne Hardering *(Department of Mathematics, TU Dresden)*
  Gradient Flows in Ambient Riemannian Manifolds Space Discretization by Geometric Finite Elements
- Laura Lauerbach *(Institute for Mathematics, University of Würzburg)*
  About a Chain of Bi-Stable Visco-Elastic Springs
- Jan Mankau *(Department of Mathematics, TU Dresden)*
  A Nonsmooth Nonconvex Descent Algorithm
- Marco Rossi *(Institute of Solid Mechanics, TU Dresden)*
  Modeling and Simulation of Electrochemical Cells under Applied Voltage
- Mathias Schäffner *(Department of Mathematics, TU Dresden)*
  Quantitative Homogenization in Nonlinear Elasticity
- Mario Varga *(Department of Mathematics, TU Dresden)*
  Stochastic Unfolding

4 Abstracts

On electrothermal feedback in organic light-emitting diodes

Matthias Liero
WIAS Berlin

Organic electronics is a future-oriented green technology using carbon-based semiconductor materials. Nowadays, devices based on organic materials can be found in everyday life e.g. in smartphone displays, photovoltaic cells, and TV screens. In addition, organic light-emitting diodes (OLEDs) have been identified as a promising alternative to conventional solid-state lighting.

However, several technological issues in the development of efficient large-area OLEDs exist. In lighting applications, a much higher brightness than in displays is required. At high power, a substantial self-heating in the device occurs, which leads to unpleasant brightness inhomogeneities. Although the role of electrothermal interplay has been recognized, the fundamental understanding of this mechanism is still missing.

This counter-intuitive pattern formation can be explained by the temperature-activated hopping transport of charge carriers in organic semiconductors, which favors thermal runaway: The electrical conductivity increases with rising temperature. At constant voltage, the electric current as well as the power dissipation increases, causing a positive feedback loop which continuously heats up the structure. Often experiments of this kind lead to the destruction of the device by thermal breakdown, if the heat cannot be dispersed into the environment.

We discuss a stationary thermistor model featuring non-Ohmic current-voltage laws. The coupled system consists of the current-flow equation for the electrostatic potential and the heat equation with Joule heating term as source. The self-heating in the device is modeled by an Arrhenius-like temperature dependency of the electrical conductivity. The non-Ohmic electrical behavior is described by a power law such that the electrical conductivity depends nonlinearly on the electric field. Notably, we allow for functional substructures with different power laws, which gives rise to a $p(x)$-Laplace-type problem with piecewise constant exponent.

The talk presents joint work with M. Bulćek (Univerzita Karlova, Prague), A. Glitzky and T. Koprucki (WIAS Berlin) and reports on experimental results of A. Fischer and R. Scholz (IAPP, TU Dresden). Support from the Einstein Center for Mathematics via MATHEON project SE2: *"Sustainable Energies: Electrothermal Modeling of Large-Area OLEDs"* is gratefully acknowledged.

Localized deformation in tensioned superelastic NiTi wire by 3D-XRD method

Petr Šittner
Institute of Physics, ASCR Prague

We investigate the propagation of macroscopic fronts of localized deformation in tensioned NiTi shape memory alloy wire by 3D synchrotron X-ray diffraction method combined with FE modelling of the localized deformation. The 3D-XRD method is used to image the elastic strains and stresses in austenite grains within the martensite band front with micrometer resolution. It is found that the local stresses in austenite grains are modified ahead of the nose cone shaped buried macroscopic interface where the martensitic transformation begins. From local stresses in individual grains we reconstruct macroscopic internal stress field in the wire which we compare with the results of FE simulations. Based on combination of experiment and simulation results we describe the topology of

the martensite band front in tensioned NiTi wire and explain the mesomechanics of its propagation at constant external stress.

Optimal control of a rate-independent evolution equation via viscous regularization

Daniel Wachsmuth
Institute for Mathematics, University of Würzburg

We study the optimal control of a rate-independent system that is driven by a convex quadratic energy. Since the associated solution mapping is non-smooth, the analysis of such control problems is challenging. In order to derive optimality conditions, we study the regularization of the problem via a smoothing of the dissipation potential and via the addition of some viscosity. The resulting regularized optimal control problem is analyzed. By driving the regularization parameter to zero, we obtain a necessary optimality condition for the original, non-smooth problem.
Joint work with Ulisse Stefanelli (Vienna) and Gerd Wachsmuth (Chemnitz)

5 Poster Abstracts

Incommensurateness in nanotwinning models of modulated martensites

Barbora Benešová
Institute for Mathematics, University of Würzburg

We study the formation of modulated martensites in ferromagnetic shape memory alloys by a mathematical model originating from the nanotwinning concept. The results show that the incommensurateness, systematically observed in experiments for the modulated phases, may be understood as a precursor effect of the intermartensitic transitions, and its appearance does not contradict the nanotwinning concept itself. The model sufficiently explains the different levels of incommensurateness reported from different experimental observations for the 14-layered and 10-layered martensites of the Ni-Mn-Ga alloy and outlines the mechanism of formation of faults in the stacking sequences of these materials. This poster presents a joint work with Miroslav Frost, Petr Sedlák, Hanuš Seiner (all Prague) and Malte Kampschulte and Christof Melcher (both Aachen).

Viscosity amplification in dilute suspensions of non-spherical particles in a Carreau matrix fluid

Jan Domurath
Leibniz-Institut für Polymerforschung Dresden

When non-spherical particles, like rods or discs, are added to a liquid, the increase in viscosity of the mixture is often described by the Lipscomb model. One important result of Lipscombs model is the prediction of a strong increase in the viscosity of the suspension with increasing aspect ratio of the filler particles. Despite the fact that this model was originally proposed for a Newtonian matrix fluid it is also applied to polymer melts filled with non-spherical particles. Such an approach completely decouples the influence of the particle shape from the non-linear properties of the suspending fluid. Yet, since polymer melts often exhibit strong non-Newtonian behaviour, e.g. shear thinning, it is to be expected that such a superposition will give a wrong prediction of the suspension viscosity. To investigate this problem we performed a numerical study of a

suspension consisting of a non-Newtonian matrix fluid and rigid spheroidal particles. In particular, we simulated different flows of a Carreau fluid around spheroidal particles with different orientations and used numerical homogenization to obtain the intrinsic viscosity of the suspension as function of applied rate of deformation, thinning exponent and aspect ratio. From the results we are able to extract the rheological coefficients A, B and C of the Lipscomb model. In the Newtonian regime simulation results coincide with Lipscombs predictions for the rheological coefficients. In the non-linear regime of the Carreau model, i.e. at high deformation rates, we found that the rheological coefficients also strongly depend on the thinning exponent. Furthermore, simulation results indicate that the rheological coefficients additionally depend on the particle orientation in the non- linear regime. This poster presents a joint work with Marina Saphiannikova, Gilles Ausias, Julien Férec, and Gert Heinrich.

Explicit Analysis of Optimal Cosserat Rotations

Andreas Fischle
Department of Mathematics, TU Dresden

Cosserat models (due to E. and F. Cosserat, 1909) are generalized continuum models which introduce additional rotational degrees of freedom. We present explicit energy-minimizing rotations for the so-called Cosserat shear-stretch energy density. The results generalize a theorem of Grioli (1940) which states that the rotation $R \in SO(n)$ which is closest to the deformation gradient $F \in GL^+(n)$ w. r. t. the euclidean distance is given by the orthogonal factor of the right polar decomposition of F. This completely new relaxed-polar mechanism of optimal Cosserat rotations sheds light on the formation of microstructure in the field of Cosserat microrotations for an isotropic geometrically nonlinear quadratic Cosserat model. A visualization of this mechanism for an idealized nanoindentation is displayed and we compare it with 3D-EBSD (electron backscatter diffraction) measurements of nanoindentations in copper single crystals which produces non-classical lattice rotation patterns in the form of counter rotations. This is joint work with P. Neff (Uni. Duisburg-Essen) and D. Raabe (Max-Planck Inst. f. Eisenforschung)

Spectral localization vs. homogenization in the random conductance model

Franziska Flegel
WIAS Berlin

We study the asymptotic behavior of the principal eigenvector and eigenvalue of the random conductance Laplacian in a large domain of $\mathbb{Z}^d$ ($d \geq 2$) with zero Dirichlet conditions. Let the conductances w be positive i.i.d. random variables, which fulfill certain regularity assumptions near zero. Then we wonder what the principal Dirichlet eigenvector looks like when the size of the domain grows to infinity. Under what conditions does it homogenize? When and how does it localize? This is partly joint work with M. Heida and M. Slowik.

EDP-convergence for delamination and a wiggly energy model

Thomas Frenzel
WIAS Berlin

We investigate parameter-dependent parabolic semi-linear PDEs which can be written as gradient flows induced by an energy functional $\mathcal{E}_\varepsilon$ and a dissipation potential $\mathcal{R}_\varepsilon$. Here ε is the microscopic

length scale. We reformulate the equation and have

$$\mathcal{E}_\varepsilon(T, u_\varepsilon(T)) + \mathcal{J}_\varepsilon(u_\varepsilon) \le \mathcal{E}_\varepsilon(0, u_\varepsilon(0)) + \int_0^T \partial_t \mathcal{E}_\varepsilon(t, u_\varepsilon(t))\, dt$$

with the total dissipation functional

$$\mathcal{J}_\varepsilon(u) := \int_0^T \mathcal{R}_\varepsilon(\dot{u}(t)) + \mathcal{R}_\varepsilon^*(-D\mathcal{E}_\varepsilon(t, u(t)))\, dt.$$

We are interested in the limit evolution as $\varepsilon \downarrow 0$. Therefore we ask for

$$\mathcal{E}_\varepsilon \xrightarrow{\Gamma} \mathcal{E}_0 \qquad \text{and} \qquad \mathcal{J}_\varepsilon \xrightarrow{\Gamma} \mathcal{J}_0.$$

We show the results for a delamination model and for a wiggly energy model. Investigation of the relation between $\mathcal{J}_0$ and $D\mathcal{E}_0$ gives rise to an effective dissipation potential $\mathcal{R}_{\text{eff}}$ in case of the wiggly energy model. In case of the delamination model we obtain a perturbed gradient flow. It is an open question if this perturbed gradient flow is in fact again an unperturbed gradient flow.

Gradient Flows in Ambient Riemannian Manifolds Space Discretization by Geometric Finite Elements

Hanne Hardering
Department of Mathematics, TU Dresden

Many variational problems have in their natural form a target manifold. We study geometric finite element discretizations of functions into a Riemannian manifold M. These reduce to standard Lagrangian finite elements if $M = \mathbb{R}^n$, and are intrinsic in the sense that the manifold is neither embedded nor approximated, and the theory is invariant under diffeomorphisms. We apply this space discretization to gradient flows after first discretizing time by an implicit Euler scheme.

About a Chain of Bi-Stable Visco-Elastic Springs

Laura Lauerbach
Institute for Mathematics, University of Würzburg

We investigate a microscopic model consisting of a chain of bi-stable viscoelastic springs. Starting from an ODE system based on an energetic approach, the vanishing-viscosity limit and the subsequent discrete-to-continuum limit show convergence to a macroscopic system with rate independent plasticity, see Mielke & Truskinovsky: "From Discrete Visco-Elasticity to Continuum Rate-Independent Plasticity: Rigorous Results.", *ARMA, 203(2):577-619.* Moreover, we consider our model under an external periodic loading and discuss some features arising by an analysis of the resulting phase diagrams.

A Nonsmooth Nonconvex Descent Algorithm

Jan Mankau
Department of Mathematics, TU Dresden

Modeling and Simulation of Electrochemical Cells under Applied Voltage

Marco Rossi
Institute of Solid Mechanics, TU Dresden

Quantitative Homogenization in Nonlinear Elasticity

Mathias Schäffner
Department of Mathematics, TU Dresden

We consider a nonlinear elastic composite with a periodic micro-structure described by the non-convex integral functional

$$I_\varepsilon(u) = \int_\Omega W\left(\frac{x}{\varepsilon}, \nabla u(x)\right) - f(x) \cdot u(x)\, dx,$$

where $u : \Omega \to \mathbb{R}^d$ is the deformation, $f : \Omega \to \mathbb{R}^d$ is an external force, $\varepsilon > 0$ denotes the size of the micro-structure, and $W(y, F)$ is a stored energy function which is periodic in y. As it is well-known, under suitable growth conditions, I_ε Γ-converges to a functional with a homogenized energy density $W_{\text{hom}}(F)$, which is given by an *infinite-cell formula*. Under appropriate assumptions on W (namely, $p \geq d$-growth from below, frame indifference, minimality at identity, non-degeneracy and smoothness in a neighborhood close to the set of rotations) and on the microstructure, we show that in a neighbourhood of rotations the homogenized stored energy function W_{hom} is of class C^2 and characterized by a *single-cell homogenization formula*. Moreover, for small data, we establish an estimate on the homogenization error, which measures the distance between (almost) minimizers u_ε of I_ε and the minimizer of the homogenized problem. More precisely, we prove that the L^2-error as well as the H^1-error of the associated two-scale expansion decays with the rate $\sqrt{\varepsilon}$. This is joint work with S. Neukamm.

Stochastic Unfolding

Mario Varga
Department of Mathematics, TU Dresden

Two-scale convergence methods have been proven to be conve- nient tools in homogenization of various equations. Problems with rapidly oscillating periodic coefficients are treated using the notion of two-scale convergence. The development of the periodic unfold- ing operator facilitated a simpler two-scale analysis of such problems by embedding sequences of oscillating functions into an appropriate two-scale space. The notion of stochastic two-scale convergence in the mean has been used to obtain homogenization results for problems in- volving oscillating random and stationary coefficients. We adapt this notion to the setting of functions defined on a discrete physical space by introducing an appropriate stochastic unfolding operator. We in- vestigate the properties of this operator which provides a basis for a simple method for convex homogenization. This is joint work with S. Neukamm.