Workshop on Mathematical Methods for Complex Phenomena

organised by

DFG SPP 2256 *Varational Methods for Predicting Complex Phenomena in Engineering Structures and Materials*

and DFG-Research Training Group 2339 *IntComSin*

Regensburg, 9–11 March 2022

Programme

In many material systems one observes complex structures which have a decisive influence on the macroscopic properties of these systems. In recent years, mathematical tools have been developed in order to understand these phenomena within models from continuum mechanics. This workshop brings together experts from two DFG funded initiatives which address these challenges: The DFG Research and Training Group 2339 Interfaces, Complex Structures, and Singular Limits and the DFG Priority Programme 2256 Varational Methods for Predicting Complex Phenomena in Engineering Structures and Materials.

Talks will take place in the lecture hall **H31**, while coffee breaks will be in the seminar room **M103**.

	Wednesday	Thursday	Friday
9:00 – 9:45		Zeppieri	Bella
9:45 – 10:15		Knopf	Badal
10:15 – 10:45		*Coffee break*	
10:45 – 11:30		Ray	Aland
11:30 – 12:00		Gärttner	Liu
12:00 – 14:00		*Lunch break*	
14:00 – 14:45	Rüland	Dondl	
14:45 – 15:30	Abels	Neuss-Radu	
15:30 – 16:00		*Coffee break*	
16:00 – 16:45	Bänsch	Schweizer	
16:45 – 17:15	Wolff-Vorbeck	Behr	
17:15 – 17:45	Hüttl	Weiss	
19:00		*Workshop dinner*	

Further informations

In the first half of the same week there is a workshop on **PDEs for Surfaces and Interfaces**, jointly organised by the DFG-Research Unit 3013 and GRK 2339.

The workshop dinner will be held at the Brauhaus am Schloss. Address: Waffnergasse 6, 93047 Regensburg.

Although, the workshop will be held in person, the talks can be followed online, via the zoom link https://uni-regensburg.zoom.us/j/62965719977?pwd=QWtiaGNOYXViUlpqQ2tMbXhBbEd1QT09, Meeting ID: 629 6571 9977, Passcode: 956582.

Detailed programme

Helmut Abels (University of Regensburg)

Wednesday, 14:45–15:30

Title: **Large Time Existence and Convergence for Thin Vibrating Rods**

Abstract: We prove existence of unique strong solutions for a nonlinear wave equation for a thin vibrating rod described by nonlinear elastodynamics. For sufficiently small thickness we obtain existence of strong solutions for large times under appropriate scaling of the initial values. In order to obtain uniform control of for small thickness we use an appropriate scaled version of Korn's inequality together with suitable estimates for the linearized wave equation. In certain cases, we even obtain a convergence rate of the three-dimensional solution to the solution of a one-dimensional linear rod equation.

Sebastian Aland, (TU Bergakademie Freiberg)

Friday, 10:45–11:30

Title: **A combined sharp/diffuse interface approach for wetting of elastic substrates**

Abstract: The interaction of an elastic substrate with liquid droplets is at small length scales dominated by surface tension forces. We present a combination of a sharp and diffuse interface model to simulate this scenario. The fluid-fluid interface is represented by a diffuse layer to regularize the contact line singularity. The solid-fluid interface is represented by a matched finite element grid and moved in the typical Arbitrary–Lagrangian–Eulerian way. As all equations are formulated in a Eulerian frame of reference, we obtain a single momentum equation including the solid and both fluid materials, which is simple to solve monolithically. We illustrate the numerical robustness of this novel method and compare it to the recent experimental and numerical results.

Rufat Badal (TU Dortmund)

Friday, 9:45–10:15

Title: **Nonlinear and Linearized Models in Thermoviscoelasticity**

Abstract: We consider a quasistatic nonlinear model in thermoviscoelasticity at a finite-strain setting in the Kelvin's-Voigt's rheology where both the elastic and viscous stress tensors comply with the principle of frame indifference under rotations. The force balance is formulated in the reference configuration by resorting to the concept of nonsimple materials whereas the heat transfer equation is governed by the Fourier law in the deformed configurations. Weak solutions are obtained by means of a staggered in-time discretization where the deformation and the temperature are updated alternatingly. Our result refines a recent work by Mielke & Roubíček [1] since our approximation does not require any regularization of the viscosity term. Afterwards, we focus on the case of deformations near the identity and small temperatures, and we show by a rigorous linearization procedure that weak solutions of the nonlinear system converge in a suitable sense to solutions of a system in linearized thermoviscoelasticity. The same property holds for time-discrete approximations and we provide a corresponding commutativity result.

[1] Mielke A., Roubíček T.: Thermoviscoelasticity in Kelvin-Voigt rheology at large strains. (2020)

Eberhard Bänsch (FAU Erlangen)

Wednesday, 16:00–16:45

Title: **The Buongiorno model for nanofluids**

Abstract: We present a mathematical model for convective transport in nanofluids including thermophoretic effects that is very similar to the celebrated model of Buongiorno. Our model, however, is thermodynamically consistent and consequently an energy estimate can be shown.

We show existence of weak solutions for the time-dependent as well as stationary problem. Moreover, an efficient numerical scheme for the time dependent problem is proposed.

For the stationary system, regularity and subsequently optimal error estimates for finite element approximations can be shown under some smallness assumptions.

Florian Behr (University of Regensburg)

Thursday, 16:45–17:15

Title: **Relaxation methods in pressure-dependent plasticity**

Abstract: Linearized plasticity is often formulated by an additive decomposition of the deformation gradient into an elastic and a plastic part and quasistatic system of equations, whose dynamics are driven by applied boundary conditions and body forces. To take pressure-dependence into account, we have to replace the associated flow-rule, which describes the evolution of the plastic part of the deformation gradient, by a non-associated flow rule. We follow an energetic approach involving a quadratic free energy and a dissipation potential, which leads in a time incremental formulation to a minimization problem of a nonconvex energy functional. To deal with the nonconvexity, it is convenient to consider the relaxation given by the quasiconvex envelope of the energy density. We introduce a lower-dimensional simplified model to avoid difficulties concerning semi-convex envelopes and present our relaxation results in this case. In particular, we give an insight in the general strategy of calculating convex envelopes and the structures of laminates, which can appear.

Peter Bella (TU Dortmund)

Friday, 9:00–9:45

Title: **Wrinkled to flat region – Γ-Convergence and beyond**

Abstract: This is a follow up on my work on the transition from flat to wrinkled regions in a uniaxially stretched thin elastic film (ARMA 2015), modeled by a non-convex singularly perturbed variational problem. Previously, I identified the leading order as well as the next order (including the right prefactor) in the expansion of the minimal energy in terms of the vanishing sheet thickness. Today I will discuss Gamma-convergence result for the next order functional as well as analysis of the limit. This is an ongoing project with Alaa Elshorbagy.

Patrick Dondl (University of Freiburg)

Thursday, 14:00–14:45

Title: **A Proof of Taylor (or Friedel) Scaling for the Critical Resolved Shear Stress**

Abstract: We prove Taylor scaling (in some contexts also known as Friedel scaling) for dislocation lines characterized by line-tension and moving by curvature under the action of an applied shear stress in a plane containing a random array of obstacles. Specifically, we show - in the sense of optimal scaling - that the critical applied shear stress for yielding, or percolation-like unbounded motion of the dislocation, scales in proportion to the square root of the obstacle density. For sufficiently small obstacle densities, Taylor scaling dominates the linear-scaling that results from purely energetic considerations as well as the two-thirds Labusch scaling, and, therefore, characterizes the dominant rate-limiting mechanism in that regime.

Joint work with L. Courte (Luxembourg) and M. Ortiz (Bonn/Pasadena).

Stefan Gärttner (FAU Erlangen)

Thursday, 11:30–12:00

Title: **Estimating permeability of real-rock micro-CT images by physics-informed neural networks**

Abstract: In recent years, convolutional neural networks (CNNs) have experienced an increasing interest for fast approximations of effective hydrodynamic parameters in porous media research. In this talk, we present a novel approach to improve permeability predictions from micro-CT scans of geological rock samples. Moreover, we justify the methodology using results from approximation theory.

A well-known method to enhance the quality of CNN predictions is the supply of additional information about the input data, leading to the field of physics-informed CNNs. Most commonly for permeability predictions from rock samples, porosity and/or (specific-) surface area are made available to the CNN as auxiliary data. However, these quantities become only loosely correlated to the target permeability for complex 3D geometries posing a poor information basis for the CNN to perform predictions.

Increasing the relevance of the additional physical information provided, we supply a highly correlated graph-network-based quantity to our CNN, namely the maximum flow value. Consequently, detailed information about confined structures dominating overall fluid flow is encoded in this additional physical input. As a result, high prediction accuracy and robustness for permeability prediction are observed across a variety of sandstone types.

Paul Hüttl (University of Regensburg)

Wednesday, 17:15–17:45

Title: **Phase-Field Approximations in Spectral Shape and Topology Optimization**

Abstract: The goal of this talk is to understand how phase-field methods can be used to optimize eigenvalues of elliptic operators on a diffuse interface level and how classical results such as the Faber–Krahn inequality can be recovered by considering the sharp interface limit. We will see that the concept of spherical symmetric decreasing rearrangements, which was used by G. Faber and E. Krahn to prove that the ball minimizes the fundamental eigenvalue of the Dirichlet Laplacian under all open sets of same volume, is very well suited to obtain a phase- field version of their famous inequality. Furthermore we want to demonstrate the flexibility of the phase-field method by discussing several numerical examples. The talk is based on joint projects with Harald Garcke (Universität Regensburg), Christian Kahle (Universität Koblenz/Landau), Patrik Knopf (Universität Regensburg) and Tim Laux (HCM Bonn).

Patrik Knopf (University of Regensburg)

Thursday, 9:45–10:15

Title: **On multiphase Cahn–Hilliard–Brinkman/Darcy models for stratified tumor growth with chemotaxis**

Abstract: We consider a multiphase Cahn–Hilliard model for tumor growth with general source terms. The multiphase approach allows us to consider multiple cell types and multiple chemical species (oxygen and/or nutrients) that are consumed by the tumor. Compared to classical two-phase tumor growth models, the multiphase model can be used to describe a stratified tumor exhibiting several layers of tissue (e.g., proliferating, quiescent and necrotic tissue) more precisely. Our model consists of a convective Cahn–Hilliard type equation to describe the tumor evolution, a velocity equation for the associated volume-averaged velocity field, and a convective reaction-diffusion type equation to describe the density of the chemical species. The velocity equation is either represented by Darcy's law or by the Brinkman equation. We further discuss the existence of global weak solutions to these models as well as the "Darcy limit" where the positive viscosities in the Brinkman equation are sent to zero.

Yadong Liu (University of Regensburg)

Friday, 11:30–12:00

Title: **On a fluid-structure interaction problem for plaque growth: cylindrical domain**

Abstract: This talk concerns a free-boundary fluid-structure interaction problem for plaque growth proposed by Yang et al. [J. Math. Biol., 72(4):973–996, 2016] with additional viscoelastic effects, which was also investigated by the authors [arXiv preprint: 2110.00042, 2021]. Compared to it, the problem is posed in a cylindrical domain with ninety-degree contact angles, which brings additional difficulties when we deal with the linearization of the system. By a reflection argument, we obtain the existence and uniqueness of strong solutions to the model problems for the linear systems, which are then shown to be well-posed in a cylindrical (annular) domain via a localization procedure. Finally, we prove that the full nonlinear system admits a unique strong solution locally with the aid of the contraction mapping principle.

Maria Neuss-Radu (FAU Erlangen)

Thursday, 14:45–15:30

Title: **Two-scale tools for homogenization and dimension reduction of porous thin layers and application to problems from elasticity**

Abstract: In this contribution we provide tools for the homogenization of thin porous layers with periodic microstructure, and dimensional reduction when the layer thickness tends to zero simultaneously with the period of the microstructure. Our multiscale methods include extension theorems which preserve also the norm of the symmetric gradient and Korn-inequalities for functions vanishing (only) on the perforated lateral boundary of the layer. To illustrate the range of applications of the developed methods a semi-linear elastic wave equation in a thin periodically perforated layer with an inhomogeneous Neumann boundary condition on the surface of the elastic substructure is treated and a homogenized, reduced system is derived. This is a joint work with Markus Gahn and Willi Jäger from IWR, University of Heidelberg.

Nadja Ray (FAU Erlangen)

Thursday, 10:45–11:30

Title: **Upscaling reactive flow and transport in evolving porous media**

Abstract: Porous media naturally exhibit a heterogeneous structure including two different spatial scales: The pore/micro-scale is the fundamental scale, on which flow and reactive transport processes take place whereas the macro-scale, i.e. the scale of the porous medium itself, is of practical relevance for many geoscientific applications. (Periodic) homogenization has been successfully applied for several decades to bridge these scales and to arrive at macroscopic (upscaled) models. However, the situation becomes more involved, if the underlying geometric structure of the porous medium alters. In this talk, we start from a pore-scale model for reactive flow and transport in a porous medium. It is composed of two distinct minerals which may dissolve and precipitate by means of chemical reactions and thus the geometric structure dynamically evolves in time and space. We give insights into the derivation of an effective micro-macro model by formal two-scale asymptotic expansion in a level-set framework. Finally, we present numerical simulations of the fully coupled micro-macro problem with application to the dissolution of calcite and dolomite.

Angkana Rüland (University of Heidelberg)

Wednesday, 14:00–14:45

Title: **On Rigidity, Flexibility and Scaling Laws for Some Matrix-Valued m-Well Problems: The Tartar Square**

Abstract: Highly non-(quasi)-convex, matrix-valued differential inclusions arise in numerous physical applications. One such example is the modelling of shape-memory alloys. In these settings, often the exact differential inclusions display a striking dichotomy between rigidity and flexibility in that

- solutions of sufficiently high regularity obey the "characteristic equations" determined by the differential inclusion, the solutions are rigid in this sense,
- while low regularity solutions are highly non-unique and hence extremely flexible.

In order to investigate this dichotomy further, in this talk, I explore the effects of regularizations in the form of singular perturbation problems with vanishing regularization strength for these differential inclusions. Motivated by applications in shape-memory alloys, I discuss the role of scaling properties in the singular perturbation strength. In particular, I the scaling behaviour of a singular perturbation problem for the Tartar square and illustrate how the structure of the underlying convex hulls results in the presented scaling laws. This is based on joint work with Jamie Taylor, Antonio Tribuzio, Christian Zillinger and Barbara Zwicknagl.

Ben Schweizer, (TU Dortmund)

Thursday, 16:00–16:45

Title: **Homogenization of domain perforations and sound absorption**

Abstract: Our analytical investigations are motivated by sound absorbing structures as you might know them from your lecture halls. Mathematically, we investigate limit equations for the Helmholtz equation in a perforated domain, where the perforation is along an interface. The analysis starts with the lowest order approximation: We find that a Neumann sieve perforation is invisible to leading order. Non-trivial transmission conditions occur for the corrector. We derive these conditions with a direct method, which relies on L^1-estimates and the study of limit measures. In a three scale geometry we derive a limit system that can explain sound absorption at perforated walls.

Patrik Weiss (University f Regensburg)

Thursday, 17:15–17:45

Title: **On the field-induced transport of magnetic nanoparticles in incompressible flow**

Abstract: In this talk we are concerned with the transport of superparamagnetic nanoparticles in flow – with the perspective of applications in magnetic drug targeting. We introduce a PDE-system which couples the momentum equation of hydrodynamics to magnetostatic equations and to the evolution equations of particle density and magnetization. Suggested by physical arguments, we consider no-flux-type boundary conditions for the magnetization equation which entails $H(\mathrm{div}, \mathrm{curl})$-regularity for magnetization and magnetic field. By a subtle approximation procedure, we establish existence of solutions in the sense of distributions in two space dimensions. We present proof of concept simulations in the 2D-case and highlight the differences to similar models in the mathematical literature.

Steve Wolff-Vorbeck (University of Freiburg)

Wednesday, 16:45–17:15

Title: **Connected coulomb columns: analysis and numerics**

Abstract: Abstract We consider a version of Gamow's liquid drop model with a short range attractive perimeter-penalizing potential and a long-range Coulomb interaction of a uniformly charged mass in $\mathbb{R}^3$. Here we constrain ourselves to minimizing among the class of shapes that are columnar, i.e., constant in one spatial direction. Using the standard perimeter in the energy would lead to non-existence for any prescribed cross-sectional area due to the infinite mass in the constant spatial direction. In order to overcome this issue we use a connected perimeter instead. We prove existence of minimizers for this connected isoperimetric problem with long-range interaction and study the shapes of minimizers in the small and large cross section regimes. For an intermediate regime we use an Ohta–Kawasaki phase field model with connectedness constraint to study the shapes of minimizers numerically. Joint work with: P. Dondl (University of Freiburg), M. Novaga (University of Pisa), S. Wojtowytsch (Texas AM University).

Caterina Zeppieri (University of Münster)

Thursday, 9:00–9:45

Title: **Γ-convergence and homogenisation of singularly-perturbed elliptic functionals**

Abstract: In this talk we analyse the limit behaviour of general elliptic functionals of Ambrosio–Tortorelli type. Under mild assumptions on the regularised volume and surface term, we show that if the volume integrand grows superlinearly in the gradient-variable, then the functionals converge to a brittle energy-functional; i.e., to a free-discontinuity functional whose surface integrand does not depend on the jump-amplitude of the limit variable. This result is achieved by showing that volume and surface terms always decouple in the limit. As an application of the abstract convergence result as above, the case of homogenisation of gradient damage models will be also discussed.