



WORKSHOP ON
MATHEMATICAL METHODS IN CONTINUUM PHYSICS AND
ENGINEERING:
THEORY, MODELS, SIMULATION



Fachbereich Mathematik
Technische Universität Darmstadt
November 6 – 7, 2019

Scientific Program Wednesday, November 6, 2019

Department of Mathematics, Lecture Hall S2|15 51

12:30 – 13:30 Registration (foyer of the lecture hall)

Opening

13:30 – 13:40 P. Neff (Essen)
Welcome address

Session 1

13:40 – 14:05 A. Mielke (Berlin)
On initial-boundary value problems for materials with internal variables or temperature dependence

14:05 – 14:30 K. Chelmiński (Warsaw)
Plasticity without safe-load conditions

14:30 – 14:55 K. Weinberg (Siegen)
Phase-field fracture models at linearized and finite deformations

14:55 – 15:20 **Coffee**

Session 2

15:20 – 15:45 P. Dondl (Freiburg)
Pinning of interfaces by localized dry friction

15:45 – 16:10 N. Kraynyukova (Frankfurt)
The impact of mRNA localization on protein distribution in neural dendrites

16:10 – 16:35 B. Kawohl (Köln)
Newton's problem of minimal resistance

Clock Tower, Lecture Hall S2|08 171

Colloquium lecture

17:30 – 18:15 H.-D. Alber
Mein akademisches Leben, geleitet durch meine Faszination für partielle Differentialgleichungen

Welcome Hotel

18:30 **Reception**

Scientific Program Thursday, November 7, 2019

Staatsarchiv**Session 3**

- 8:30 – 8:55 E. Khruslov (Kharkov)
2D model of photonic metamaterial with preassigned gaps in spectrum
- 8:55 – 9:20 R. J. Knops (Edinburgh)
Generalisations of Filon's Construct
- 9:20 – 9:45 K. Hutter (Zürich)
Beyond Power Law Fluids
- 9:45 – 10:10 **Coffee**

Session 4

- 10:10 – 10:35 P. Neff (Essen)
Identification of scale-independent material parameters in the relaxed micromorphic model through model-adapted first order homogenization
- 10:35 – 11:00 A. Schlömerkemper (Würzburg)
About dissipative solutions in an evolutionary system for magnetoviscoelastic materials
- 11:00 – 11:25 R. Picard (Dresden)
On Abstract Friedrichs Systems and Some of their Applications
- 11:25 – 11:45 **Coffee**

Session 5

- 11:45 – 12:10 P. Zhu (Shanghai)
Viscosity solutions to a model for solid–solid phase transitions driven by material forces
- 12:10 – 12:35 H. Abels (Regensburg)
Sharp Interface Limit for the Allen-Cahn Equation with a Contact Angle
- 12:35 – 13:00 T. Sarantuya (Ulaanbaatar)
Aktivitäten und Beitrag zur mathematischen Bildung an der Mongolischen Universität für Wissenschaft und Technologie

End of the workshop

ABSTRACTS

Sharp Interface Limit for the Allen-Cahn Equation with a Contact Angle

Helmut Abels
Universität Regensburg

We consider the sharp interface limit of a coupled Stokes/Allen-Cahn system, when a parameter $\varepsilon > 0$ that is proportional to the thickness of the diffuse interface tends to zero, in a two dimensional bounded domain. For sufficiently small times we prove convergence of the solutions of the Stokes/Allen-Cahn system to solutions of a sharp interface model, where the interface evolution is given by the mean curvature equation with an additional convection term coupled to a two-phase Stokes system with an additional contribution to the stress tensor, which describes the capillary stress. To this end we construct a suitable approximation of the solution of the Stokes/Allen-Cahn system, using three levels of the terms in the formally matched asymptotic calculations, and estimate the difference with the aid of a suitable refinement of a spectral estimate of the linearized Allen-Cahn operator. This is a joint-work with Maximilian Moser.

Plasticity without safe-load conditions

Krzysztof Chelmiński

Faculty of Mathematics and Information Science

Politechnika Warszawska

Systems of equations describing an inelastic response of metals, with fundamental assumption of small deformations, consist of linear partial differential equations coupled with nonlinear differential inclusions (or ordinary differential equations) for the vector of internal variables. One of the main assumptions needed in known existence theories is so-called safe-load condition. This kind of assumption is an indirect assumption on regularity of data. Our main goal is to present a method to obtaining existence of solutions, where the safe-load condition can be replaced by an assumption on some norms of the Neumann boundary data and the external force acting on the considered material.

Pinning of interfaces by localized dry friction

Patrick Dondl
Universität Freiburg

We consider a differential inclusion to model the propagation of an interface, e.g., a phase boundary, in an environment with obstacles. The interaction of the interface with the obstacles is governed by a localized dry friction. The model implies that energy has to be expended to pass across an obstacle. Hence, the interface becomes arrested until enough curvature is accumulated such that it is energetically more favorable to pass across the obstacle. The treatment of our model in the context of pinning and depinning requires a comparison principle. We prove this property and hence the existence of viscosity solutions. Moreover, under reasonable assumptions, they are equivalent to weak solutions. Our main results asserts that for obstacles distributed according to a Poisson point process, interfaces become pinned, leading to the emergence of a rate-independent hysteresis.

Joint work with Luca Courte (Freiburg) and Ulisse Stefanelli (Vienna).

Beyond Power Law Fluids

Kolumban Hutter
Bergstrasse 5, Zürich

The classical viscous fluid model is the Navier-Stokes fluid, in which the constitutive stress tensor is linearly related to the stretching tensor with possibly temperature dependent viscosity. The most popular extensions of this for density preserving fluids are constitutive relations in which the strain rate deviator and the constitutive stress are affine to one another with a scalar coefficient that depends on the second invariant of the stress deviator, most often in form of a power law. The most general class of such viscous isotropic constitutive laws are the Reiner-Riwlin fluids, in which the stretching deviator is expressed as a second order polynomial of the stress deviator with coefficient functions that are – apart from any temperature dependence – functions of the second and third invariant of the stress deviator.

It is shown that any extension beyond the classical affinity between stress and strain-rate deviators must be of full Reiner-Riwlin type. Moreover, experimental arrangements are sketched by which the two phenomenological functions of the Reiner-Riwlin law can in principle be experimentally determined. However, today's machines are still not flexible enough that these functions could be identified.

Newton's problem of minimal resistance

Bernd Kawohl
Mathematisches Institut
Universität zu Köln

Newton's problem of minimal resistance is one of the oldest problems (1685) in the calculus of variations. In the talk I present the problem and Newton's "solution" and I survey some results that were obtained more than 200 years later. Numerical results lead to unexpected conjectures.

2D model of photonic metamaterial with preassigned gaps in spectrum

Evgen Khruslov

B. Verkin Institute for Low Temperature Physics and
Engineering of NASU, Kharkov, Ukraine

We study the Maxwell operator in the two-dimensional dielectric medium with small perfectly conducting inclusions which are periodically distributed with a small period ε . The media of such a structure are typical for the photonic metamaterials, that is for the artificial composite materials with prescribed electromagnetic properties.

The spectrum of the Maxwell operator in such a medium is continuous and has a band-gap structure, but the gaps in spectrum can be absent. On the other hand, for applications in the radio engineering it is important to be able to design photonic materials whose spectra have the gaps with preassigned locations.

For this purpose we consider the trap-like inclusions in the form of cylindrical shells with thin slots along generatrices.

We prove that for a sufficiently small period ε the spectrum of the associated Maxwell operator has a finite number of gaps with the edges which converge to the prescribed points as $\varepsilon \rightarrow 0$. We establish a one-to-one correspondence between parameters of the trap-like inclusions and the edges of the limiting spectrum. In the proof we apply methods of the homogenization theory, of the Floquet-Bloch theory and the min-max theorems.

Generalisations of Filon's Construct

Robin J. Knops

School of Mathematical and Computing Sciences
and the Maxwell Institute of Mathematical Sciences
Heriot-Watt University, Edinburgh

Filon's construct (1921) originally relates two-dimensional dislocation solutions to the difference between solutions for two sets of moduli to the same plane linear elastostatic problem. The construct, however, is considerably broader in potential scope and indeed its history, which is briefly reviewed, antedates Filon's contribution. Here, we first sketch how cut-and-weld operations may be used to motivate and unify extension of the construct to three dimensional anisotropic nonhomogeneous static and dynamic linear coupled theories and then continue by rigorously deriving the various interrelationships. In addition, a further link with Ericksen's notion of universal solutions is explained. Selected examples illustrate aspects of these developments

The work is mainly joint with Professor Amit Acharya, Carnegie-Mellon University.

The impact of mRNA localization on protein distribution in neural dendrites

Fonkeu Y*, Kraynyukova N*, Hafner AS*, Kochen L, Sartori F, Schuman EM,
Tchumatchenko T
Max Planck Institute for Brain Research, Frankfurt

Each location of neural dendrites needs a sufficient amount of proteins for signal transmission and memory storage. How neurons meet this demand is currently poorly understood. A well-established basic model for dendritic protein dynamics is represented by a drift-diffusion equation that describes how the processes of transport, degradation, and production affect protein availability at a specific dendritic location at a given point of time. This model, however, is inconsistent with a series of recent experimental observations on protein dynamics including, for example, fast local protein increase after synaptic stimulation.

Proteins are synthesized from their corresponding mRNA molecules. Previous models for protein dynamics assume a central somatic source for protein production. Recent experimental work has shown, however, that mRNA of many proteins are abundant in neural dendrites and that protein synthesis also can take place locally. In our recent work [1], we combined theoretical and experimental approaches to analyze the validity of the central somatic source assumption. We argue that the coupling of protein dynamics equation to mRNA availability in dendrites can easily explain a set of dynamical phenomena not captured by the previous models. We show how somatic and dendritic mRNA sources shape the dendritic protein distribution in space and time. To test our model, we analyze the high-resolution fluorescence data for CaMKII α mRNA and protein molecules in a cultured hippocampal neuron, an important protein involved in synaptic transmission. From this data, we determined transport parameters based on our model predictions and found them to be in line with experimentally reported values. Using these parameters, we show that the model accurately explains a set of dynamical experimental observations for the protein CaMKII α . Finally, we provide a web-based applet to explore protein and mRNA dynamics for other molecules of interest.

References

- [1] Fonkeu Y*, Kraynyukova N*, Hafner AS*, Kochen L, Sartori F, Schuman EM, Tchumatchenko T,
How mRNA Localization and Protein Synthesis Sites Influence Dendritic Protein Distribution and Dynamics, NEURON 103, 1109–1122, 2019. *equal contribution

On initial-boundary value problems for materials with internal variables or temperature dependence

Alexander Mielke

Weierstraß-Institut für Angewandte Analysis und Stochastik
and Humboldt-Universität zu Berlin

Materials with memory can be described mathematically by *initial-boundary value problems for constitutive equations with internal variables* as is described in the monograph [Alb98]. In these equations nonlinearities arise in several ways. Firstly, the condition of material frame indifference leads to geometric nonlinearities [MaM09], secondly the local condition of non-selfinterpenetration leads to constitutive nonlinearities [KZM10, MiR16]. Finally viscous flow laws in plasticity with yield stress are obvious nonlinear and even nonsmooth, cf. [Alb98, MRS18].

In this talk we describe recent work with Tomas Roubicek [MiR19] concerning the coupling of finite-strain visco-elasticity with temperature effects. New nonlinearities arise through the thermomechanical and the viscous heating. Solutions are constructed by a regularized incremental scheme, where it is crucial to use a generalized Korn's inequality developed at TU Darmstadt [Nef02, Pom03].

- [Alb98] H.-D. ALBER. *Materials with Memory*, volume 1682 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1998.
- [KZM10] D. KNEES, C. ZANINI, and A. MIELKE. Crack growth in polyconvex materials. *Physica D*, 239, 1470–1484, 2010.
- [MaM09] A. MAINIK and A. MIELKE. Global existence for rate-independent gradient plasticity at finite strain. *J. Nonlinear Sci.*, 19(3), 221–248, 2009.
- [MiR16] A. MIELKE and T. ROUBÍČEK. Rate-independent elastoplasticity at finite strain and its numerical approximation. *Math. Models Meth. Appl. Sci.*, 26(12), 2203–2236, 2016.
- [MiR19] A. MIELKE and T. ROUBÍČEK. Thermoviscoelasticity in Kelvin-Voigt rheology at large strains. arXiv 1903.11094, WIAS preprint 2584, 2019.
- [MRS18] A. MIELKE, R. ROSSI, and G. SAVARÉ. Global existence results for viscoplasticity at finite strain. *Arch. Rational Mech. Anal.*, 227(1), 423–475, 2018.
- [Nef02] P. NEFF. On Korn's first inequality with non-constant coefficients. *Proc. Roy. Soc. Edinburgh Sect. A*, 132, 221–243, 2002.
- [Pom03] W. POMPE. Korn's first inequality with variable coefficients and its generalization. *Comment. Math. Univ. Carolinae*, 44(1), 57–70, 2003.

Identification of scale-independent material parameters in the relaxed micromorphic model through model-adapted first order homogenization

Patrizio Neff
Fakultät für Mathematik
Universität Duisburg-Essen

We rigorously determine the scale-independent short range elastic parameters in the relaxed micromorphic generalized continuum model for a given periodic microstructure. This is done using both classical periodic homogenization and a new procedure involving the concept of apparent material stiffness of a unit-cell under affine Dirichlet boundary conditions and Neumann's principle on the overall representation of anisotropy. We explain our idea of "maximal" stiffness of the unit-cell and use state of the art first order numerical homogenization methods to obtain the needed parameters for a given tetragonal unit-cell.

On Abstract Friedrichs Systems and Some of their Applications

Rainer Picard
Technische Universität Dresden

Many models of mathematical physics share a common form

$$\partial_t V + AU = F,$$

where ∂_t denotes time-differentiation and A is a maximal accretive linear operator, F a given source term. Indeed, in standard cases A is simply skew-selfadjoint in an underlying real Hilbert space H . The unknowns U, V are here linked by a so-called material law

$$V = \mathcal{M}U.$$

In a number of studies it has been illustrated, that this simple framework is indeed suitable for a large number of complex applications including even time-delay problems and fractional time derivatives. A typical and simple case, which we shall focus on here is

$$\mathcal{M} = M_0 + \partial_t^{-1} M_1, \tag{0.1}$$

where M_0, M_1 are continuous linear operators in H , in particular, M_0 is selfadjoint. The operator ∂_t^{-1} appearing here is forward causal time-integration, which can be properly realized in a weighted Hilbert space setting. In this case a basic well-posedness constraint for material laws of the form (0.1) is that

$$\rho M_0 + M_1 \geq c_0 > 0 \tag{0.2}$$

holds for some real number c_0 and all sufficiently large positive $\rho \in \mathbb{R}$.

For A skew-selfadjoint these systems can be transformed into operator equations of the form

$$1 + \mathcal{A},$$

where now \mathcal{A} is skew-selfadjoint. Since the classical Friedrichs systems can also be brought into this formal shape, we speak of abstract Friedrichs systems. With the skew-selfadjointness of A playing a central role, we present a number of tools, useful for modeling concrete problems, to construct such operators. These tools as well as the utility of the general setting are illustrated with various applications from mathematical physics.

Aktivitäten und Beitrag zur mathematischen Bildung an der Mongolischen Universität für Wissenschaft und Technologie

Sarantuya Tsedendamba
Mongolian University of Science and Technology, Ulaanbaatar, Mongolia

Der mehrjährigen Zusammenarbeit gewidmet zum 70. Geburtstag von Professor Hans-Dieter Alber der TU Darmstadt hat man an der Mongolischen Universität für Wissenschaft und Technologie die Bedeutung des Professorenaustausches und der Forschungsaufenthalte der mongolischen Mathematikprofessoren an den Deutschen Hochschulen und Universitäten unterstützt durch den DAAD zur Entwicklung der Mathematik in der Mongolei besonders hervorgehoben.

Auch an die mongolischen Mathematiker, die in Deutschland promoviert haben und in der Mongolei erfolgreich im akademischen Bereich arbeiten oder arbeiteten nachgedacht und betont worden durch folgende Aktivitäten:

- Organisation der Deutsch-Mongolischen Mathematiker Konferenzen
- Organisation der CIMPA Sommerschulen in partiellen Differentialgleichungen in der Mongolei
- Die Vertiefung und die Unterstützung der Zusammenarbeit mit den Professoren der MUWT und der TU Darmstadt auf Förderung vom DAAD
- Studentenaustausches im Rahmen der Zusammenarbeit mit der TU Darmstadt und DSH Prüfung.

About dissipative solutions in an evolutionary system for magnetoviscoelastic materials

Anja Schlömerkemper
Universität Würzburg

We study a model for magnetoviscoelastic materials that is a system coupling the incompressible Navier-Stokes equations, an evolutionary equation for the deformation and the Landau-Lifshitz-Gilbert equation. In this talk I will address the question of global in time existence with general initial data and present our existence result of dissipative solutions in two and three dimensions. This is joint work with Martin Kalousek.

Phase-field fracture models at linearized and finite deformations

Kerstin Weinberg
Universität Siegen

The basic idea of phase-field simulations of fracture is to mark the material's state by an order parameter z , with $z = 0$ indicating the intact solid and $z = 1$ the broken state. While cracks are actually sharp two-dimensional hypersurfaces, the use of a continuous order parameter field -the phase field- regularizes the sharp material discontinuities with smooth transitions between broken and unbroken regions.

The evolution of the phase-field follows an evolution equation where the driving forces of crack growth are derived from an energy minimization principle, typically based on an Ambrosio-Tortorelli type functional. Modifications allow accounting for the no-healing irreversibility constraint of crack evolution and, especially important, for the asymmetry of fracture, i.e., the fact that cracks only grow under tensile loadings but not under compression. Further modifications consider the evolution problem at finite strains using energy densities, which are polyconvex functions of the deformation, [1].

Here we discuss different decompositions of the elastic energy and the pros and cons of variational and ad hoc formulations for the crack driving forces, cf. [2, 3]. The latter may base on positive principal stresses or strains for example. We compare different models in linearized and in finite elasticity and present recent results on the mathematical analysis for a phase-field model at finite strains, where we formulate the phase-field with energy densities in terms of the modified invariants of the right Cauchy-Green strain tensor. To illustrate the capability of a phase-field fracture approach we present finite element simulations of brittle fracture in a Brazilian test specimen and compare it to our experimental results. The main challenge of such fracture simulations is, that it requires the ability of a numerical method to predict crack nucleation and fracture without stress concentration at a notch or at an initial crack.

- [1] Thomas, Marita and Carola Bilgen and Kerstin Weinberg. Phase-Field Fracture at Finite Strains Based on Modified Invariants: A Note on its Analysis and Simulations. *GAMM-Mitteilungen* 40(3): 207–237, 2018
- [2] Carola Bilgen and Kerstin Weinberg. On the crack-driving force of phase-field models in linearized and finite elasticity. *Computer Methods in Applied Mechanics and Engineering*, 353: 348-372, 2019
- [3] Carola Bilgen and Stefanie Homberger and Kerstin Weinberg. Phase-field fracture simulations of the Brazilian Splitting Test. accepted for publication in: *International Journal of Fracture*, 2019

Viscosity solutions to a model for solid-solid phase transitions driven by material forces

Peicheng Zhu
College of Science, Shanghai University, China

A phase-field model is formulated to describe structural phase transformations that are driven by material forces, in solid materials, e.g., shape memory alloys. This model is a nonlinear degenerate parabolic equation of second order and its principal part is not in divergence form in multi-dimensional case. We shall prove the global existence of viscosity solutions to an initial-boundary value problem for this model.

LIST OF PARTICIPANTS

Abels, Helmut	helmut.abels@mathematik.uni-regensburg.de
Alber, Hans-Dieter	alber@mathematik.tu-darmstadt.de
Celik, Aday	celik@mathematik.tu-darmstadt.de
Chełmiński, Krzysztof	chel@mimuw.edu.pl
Dondl, Patrick	patrick.dondl@mathematik.uni-freiburg.de
Ebenfeld, Stefan	sebenfeld@deloitte.de
Eiter, Thomas	eiter@mathematik.tu-darmstadt.de
Farwig, Reinhard	farwig@mathematik.tu-darmstadt.de
Giesselmann, Jan	giesselmann@mathematik.tu-darmstadt.de
Hutter, Kolumban	hutter@vaw.baug.ethz.ch
Kawohl, Bernd	kawohl@math.uni-koeln.de
Khruslov, Evgen	khruslov@ilt.kharkov.ua
Knops, Robin	R.J.Knops@hw.ac.uk
Kraynyukova, Nataliya	nataliya.kraynyukova@brain.mpg.de
Liess, Otto	liess.otto@gmail.com
Mielke, Alexander	alexander.mielke@wias-berlin.de
Neff, Patrizio	patrizio.neff@uni-due.de
Picard, Rainer	rainer.picard@tu-dresden.de
Racke, Reinhard	reinhard.racke@uni-konstanz.de
Sarantuya, Tsedendamba	saraa@must.edu.mn
Schlömerkemper, Anja	anja.schloerkemper@mathematik.uni-wuerzburg.de
Speck, Frank-Olme	fospeck@gmail.com
Weinberg, Kerstin	kerstin.weinberg@uni-siegen.de
Wendland, Wolfgang	wendland@mathematik.uni-stuttgart.de
Zacharenakis, Dimitrios	zacharenakis@mathematik.tu-darmstadt.de
Zahn, Ingo	ingo.zahn@o2mail.de
Zhu, Peicheng	pczhu@t.shu.edu.cn