Mathematisches Forschungsinstitut Oberwolfach

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Numerik von Mikrostrukturen

June 17th – June 23rd 2001

The wide-spread topics of the second half-meeting under the title numerics of microstructures ranged from small geometric details to advanced materials. The simulations addressed models on a microscopic level and its resulting macroscopic phenomena and so numerical and analytical homogenization was one main concern with applications to fluid mechanics (cf. W. Jägers talk) to crystal physics (cf. M. Luskins' talk) or plasticity (cf. K. Hackl's talk). One major issue is the resolution of the microscopic structure in case this is nonperiodic addressed by several speakers (Y. Efendiev, S. Sauter, F. Bornemann, P. Plecháč, Z. Chen). In the heart of the meeting were algorithmic questions (Can we compute the global minimizer?) linked with modeling aspects (Is quasiconvexification the ultimate goal?) and the design of efficient algorithms (multigrid and adaptive mesh-design).

Schedule of the meeting

Monday

9.15 – 9.10	*Yalchin Efendiev*: Modeling and Computation of some Nano-Size Microstructures
11.00 – 12.00	*Wolfgang Hackbusch*: The Hierarchical Matrix Approach Applied to the divΔ^{-1}grad Operator
16.00 – 17.00	*Willi Jäger*: Laws at Interfaces and Rough Boundaries for Navier-Stokes-Flow
17.15 – 18.15	*Klaus Hackl* On the Calculation of Microstructures for Inelastic Materials Using Relaxed Energies

Tuesday

9.15 – 10.15	*Bo Li*: Numerical Modeling of Martensitic Microstructure near a Laminate-single Variant Interface
11.00 – 12.00	*Zhiping Li*: Mesh Transformation Method and Computation of Needly-like Microstructures
16.00 – 17.00	*Mitchell Luskin*: Indentation and Shape Memory of a Martensitic Thin Film
17.15 – 18.15	*Noel J. Walkington*: Mathematical Models of Fluids with Structure

Wednesday

9.00 – 10.00	*Georg Dolzmann*: Evolution of Viscoelastic Solids with Microstructure – Existence and Approximation
10.00 – 11.00	*Ulrich Weikard*: Numerics of the Cahn-Hilliard Model
11.30 – 12.30	*Zhiming Chen*: A Mixed Multiscale FEM for Elliptic Problems with Oscillating Coefficients
13.45 – 18.00	Hiking tour

Thursday

9.00 – 10.00	*Stefan Sauter*: A Posteriori Error Estimation for Elliptic PDEs on Complicated Domains
10.00 – 10.30	*Sören Bartels*: Numerical Analysis of some Multi-Well Problems
11.15 – 12.15	*Christof Eck*: A Two-Scale Method for Liquid-Solid Phase Transitions with Dentritic Microstructure
16.00 – 17.00	*Folkmar Bornemann*: Multigrid Homogenization
17.15 – 18.15	*Andreas Prohl*: Numerical Analysis of Nematic Liquid Crystals

Friday

9.15 – 10.15	*Tomas Roubíček*: Microstructure Evolution
10.45 – 11.45	*Petr Plecháč*: Relaxation in Finite-Temperature Micromagnetism
11.45 – 12.15	Discussion
12.15 – 12.30	Closing Remarks

Abstracts

Numerical Analysis of some Multi-Well Problems

Sören Bartels (University of Kiel)

The mathematical model of phase transitions in crystalline solids leads to the minimization of non-quasiconvex energy functionals over a space of admissible deformations. For the case of gradients and mutually compatible energy wells we show that finite element minimizers exhibit branching structures whose geometry depends on growth conditions of the employed energy density. This is a result of joint work with Andreas Prohl. In the second half of the talk error estimates for the adaptive Young measure approximation in scalar non-convex variational problems are derived. Combined with an active set strategy of Carstensen and Roubíček they yield an efficient algorithm for the numerical approximation of measure valued solutions.

Multigrid Homogenization

Folkmar Bornemann (University of Munich)

We survey different methods for upscaling within a multigrid cycle and propose a new method guided by the theory of H-convergence by Murat/Tartar.

A Mixed Multiscale FEM for Elliptic Problems with Oscillating Coefficients

Zhiming Chen (Chinese Academy of Sciences, Beijing)

The recently introduced multiscale finite element method [19,18] for solving elliptic equations with oscillating coefficients is designed to capture the large scale structure of the solutions without resolving all the fine scale structures. Motivated by the numerical simulation of flow transport in highly heterogeneous porous media, we propose a mixed multiscale finite element method with an over-sampling technique for solving second order elliptic equations with rapidly oscillating coefficients. The multiscale finite element bases are constructed by locally solving Neumann boundary value problems. We provide a detailed convergence analysis of the method under the assumption that the oscillating coefficients are locally periodic. While such a simplifying assumption is *not* required by our method, it allows us to use homogenization theory to obtain the asymptotic structure of the solutions. Numerical experiments are carried out for flow transport in a porous medium with a random log-normal relative permeability to demonstrate the efficiency and accuracy of the proposed method.

Evolution of Viscoelastic Solids with Microstructure – Existence and Approximation

Georg Dolzmann (University of Maryland, College Park)

We consider the system of viscoelasticity,

$$u_{tt} = \operatorname{div}\big(\sigma(Du) + Du_t\big) \text{ in } \Omega \times (0,\infty)$$

for an elastic deformation $u : \Omega \subset \mathbb{R}^n \to \mathbb{R}^m$ subject to suitable boundary and initial conditions. The potential Φ of the elastic stress σ only needs to satisfy the following conditions:

(H1) $\Phi \in C^2$;
(H2) $c|F|^p - C \le \Phi(F) \le C\big(|F|^p + 1\big)$ and $|\sigma(F)| \le C\big(|F|^{p-1} + 1\big)$;
(H3) $\big(\sigma(F_1) - \sigma(F_2)\big) : (F_1 - F_2) \ge -K|F_1 - F_2|^2$, $K > 0$.
In particular, (H3) is satisfied if σ is monotone or globally Lipschitz continuous. In this situation, the following theorem holds:

Theorem: There exists a weak solution u of the system with

$$u \in L^\infty(\mathcal{A}) \cap W^{1,\infty}(L^2) \cap W^{1,2}_{\mathrm{loc}}(W^{1,2}) \cap W^{2,2}_{\mathrm{loc}}(W^{-1,p'}).$$

Moreover, if σ is globally Lipschitz continuous, then u is unique.

Adapting the implicit time discretization scheme in the proof of this theorem, one easily obtains the existence of a finite element approximation of the system that combines a discontinuous Galerkin approximation in time with Courant elements in space. The following a priori error estimate can be deduced similarly to the uniqueness proof for the continuous system:

Theorem: Assume that the time step-size k is small enough, that U_j is the finite element approximation with discrete velocity V_j and that $e_j = u(t_j) - U_j$ and $\delta_j = u_t(t_j) - V_j$ denote the errors in the displacement and the velocity, respectively. Then

$$\max_{j=1,\dots,N} \|e_j\|^2 + \sum_{j=1}^{N} k_j \big(\|\delta_j\|^2 + \|De_j\|^2\big) \le \big(a_0 + \mathcal{A}(T) + \mathcal{R}(T)\big) \exp(cT),$$

where a_0, $\mathcal{A}(T)$ and $\mathcal{R}(T)$ are of order $\mathcal{O}(h^2 + k^2)$ if the solution u is sufficiently smooth and the triangulations are only refined in time, but not coarsened.
This is joint work with G. Friesecke (Warwick) and C. Carstensen (Vienna).

A Two-Scale Method for Liquid-Solid Phase Transitions with Dendritic Microstructure

Christof Eck (University Erlangen-Nürnberg)

In many liquid–solid phase transitions, a dendritic microstructure of the solid–liquid interface can be observed. The microstructure arises from an instability of a "regular" phase interface in an undercooled melt with respect to small perturbations. Proper models for its evolution are either sharp interface models including curvature effects or phase field models. However, the scale of the dendritic structure is in general too small to be resolved by a global grid in a numerical computation.

Here, a two–scale phase field model for phase transitions with dendritic microstructure in binary mixtures is presented. The model consists of a macroscopic heat equation to be solved on the domain under consideration, and, at each point of this macroscopic domain, of a microscopic isothermal phase transition problem to be solved on an upscaled local periodicity cell. The model is derived by homogenization of a phase field model for binary mixtures under the assumption of a periodic initial distribution of solid kernels and of a suitable scaling for solute diffusivity, interfacial energy and the parameters of the phase field model. Both the original problem and the two–scale model are discretized by a conforming finite element method with respect to the space variables and an implicit Euler method with respect to the time variable. For both models a priori error estimates are presented and compared.

Modeling and Computation of some Nano-Size Microstructures

Yalchin Efendiev (University of Minneapolis)

The nano-size microstructures are grown recently with applications in material synthesis and growth control of nanodroplets. I will talk how we simultaneously model and compute the growth of heterogeneous particles and study the evolution of their internal structure. Sectional and Monte-Carlo approaches will be discussed.

The Hierarchical Matrix Approach Applied to the $div\Delta^{-1}grad$ Operator

Wolfgang Hackbusch (Max-Planck-Institute for Mathematics)

As a part of the magnetisation energy in micromagnetism one has to compute $\xi_{m^3}(Du)^2$ for the solution u of $Du + div\underline{m} = 2$, where $supp\,\underline{m}\,\underline{c}\,\Omega$. In particular, if $\underline{m}$ is discretised by piecewise constant finite elements, one has to evaluate the integral operator with the kernel $div_x\, div_y \frac{1}{(t-y)}$. Since this kernel is singular, a suitable regularisation has to be applied. The arising dense stiffness matrix can be replaced by a hierarchical matrix, so that the overall work is almost proportional to $n=$ dimension of the finite element space.

On the Calculation of Microstructures for Inelastic Materials Using Relaxed Energies

Klaus Hackl (University of Bochum)

A general variational formulation for materials with internal variables is preserved. For the time-incremental problem this formulation allows to derive a reduced elastic potential along with an update-procedure for the internal variables. The reduced potentials are calculated for two models of finite-strain elasto-plasticity (single-slip, v. Mises). The potentials turn out to be not rank-one convex. For the single slip model the occurrence of microstructures is demonstrated numerically. A rank 1-relaxation of the potential is calculated numerically using sequential quadratic programming. Several examples are shown and the results discussed.

Laws at Interfaces and Rough Boundaries for the Navier-Stokes-Flow

Willi Jäger (University of Heidelberg)

A survey is given covering the results of asymptotic analysis for a problem arising in flow along rapidly oscillating boundaries or in a partially porous medium. The transmission conditions connecting free flow and filtration flow in a porous medium are discussed and effective boundary conditions on an approximating "smooth" boundary replacing a rough one are derived. The effective terms and quantities can be numerically computed, errors of approximations are estimated.
The results were obtained in joint work with A. Mikelič and N. Neuß.

Numerical Modeling of Martensitic Microstructure near a Laminate-single Variant Interface

Bo Li (University of Maryland)

We report results of numerical modeling of martensitic microstructure near a laminate-single variant interface in a Copper-Aluminium-Nickle single crystal. We construct continuum models for the microstructure using the geometrically nonlinear theory of martensite. We develop numerical methods that combine the finite element discretization and various kinds of optimization algorithms. We show the graphics of the computed Cauchy-Green strain field which are found to agree with experiment to a great extent. Finally, we compare our results in the context of atomistic dislocations and surface energy.
This is a joint work with Michell Luskin.

Mesh Transformation Method and Computation of Needly-like Microstructures

Zhiping Li (University of Peking)

In this talk, we study the mesh transformation and its application to the computation of needle-like microstructures near the austenite-finely twinned martensite interface.

The idea of the mesh transformation method is to involve the mesh distribution into the minimization procedure so that the mesh can align with the twin boundaries and thus essentially avoid the pollution of the mesh to the finite element approximations, which is known to be responsible to the poor numerical results produced by the classical finite element approximations. Furthermore, the application of the mesh transformation method makes it possible for us to get numerical results with reasonable precision on a coarse mesh.

While the energy minimizing sequences take a crucial role in the computation of Young measures which give the the probability distribution of the microstructure, the local minimizers of the energy can also be of great importance, especially in the case, as is in this talk, when the profile of the needles near the austenite-finely twinned martensite interface is under consideration. In fact, it is such local minimizers, which contain the detailed information of the needles near the austenite-finely twinned martensite interface, that we are trying to compute with the mesh transformation method.

Indentation and Shape Memory of a Martensitic Thin Film

Mitchell Luskin (University of Minnesota)

On the numerical modeling of the indentation and shape memory of a martensitic thin film. We propose a computational model for a stress-induced martensitic phase transformation of a single-crystal thin film by indentation and its reverse transformation to austenite by heating. Our model utilizes a surface energy that allows sharp interfaces with finite energy and a penalty that forces the film to lie above the indenter and undergo a stress-induced austenite-to-martensite phase transformation. We introduce a method to stochastically nucleate the martensite-to-austenite phase transformation during heating.

Relaxation in Finite-Temperature Micromagnetism

Petr Plecháč (University of Delaware)

Recent advances in applications of ultrathin magnetic films pointed out the importance of thermal fluctuations in micromagnetic models. The standard Landau-Lifschitz theory,

which has been successfully applied to modeling of magnetic microstructures does not allow to incorporate the thermal noise in a systematic way. In the joint work with Prof. M. A. Katsoulakis (University of Massachusetts, Amherst) we derive macroscopic description of ferromagnetic material at a positive finite temperature. This new formulation describes the most-probable equilibrium macrostates that yield a coherent deterministic large-scale picture varying at the size of the domain as well as it captures the effect of random spin fluctuation caused by the thermal noise. The averaged formulation is more suitable for numerical treatment as it does not require resolution of extremely fine features of the solution. Similar approach has been used in numerical treatment of the relaxed Landau-Lifschitz energy functional. We also discuss relation to this relaxation in the zero-temperature limit of our variational problem.

Numerical Analysis of Nematic Liquid Crystals

Andreas Prohl (University of Kiel)

Nematic Liquid crystals are ordered fluids composed of elongated rod-like molecules. Their description is by Leslie-Ericksen's theory, for d, u, p the director, velocity and pressure field. Recently presented numerical schemes and their analyses (Liu & Walkington) use Hermite-type finite elements, unrealistic assumptions on regularities, and they prove convergence results where upper-bounds blow up w.r.t. a penalization parameter that controls conservation of the length of molecules (i.e., $|d| = 1$). In the talk, we propose and analyze a time-splitting method combined with Lagrange-type finite elements for efficient computation of the solution. Convergence estimates do not show blow up w.r.t. the penalization parameter that is identified as a numerical quantity.

Microstructure Evolution

Tomas Roubíček (Charles University, Prague)

Standard evolution models of isothermal martensitic transformation in shape-memory alloys on a "microscopical" level are based on the viscosity-like and/or capillarity-like equations of the type

$$\varrho\ddot{u} - \mathrm{div}(\sigma(\nabla u)) + \nu(-1)^n\Delta^n\dot{u} + \mu(-1)^m\Delta^m u = f, \quad u(0) = u_0, \quad \dot{u}(0) = u_1,$$

with the stress response σ nonmonotone. Some arguments exit to indicate that this class of models cannot serve well to produce (at least approximately) rate-independent hysteretic response with amount of dissipated energy controlled as a phenomenological parameter independent of σ, as desirable to fit with experimental evidence. A solution by augmentation of the above class of equation by the term $\mathrm{div}(\mathrm{signum}(\lambda'(\nabla u)\nabla\ddot{u})\lambda'(\nabla u))$ with λ a suitable order parameter (only one suffices in a two-well situation) is offered. Alternative variant for a "mesoscopical-level" model playing with Young measures is outlined, too. Modification for the case of ferromagnetism is possible, too.

A Posteriori Error Estimation for Elliptic PDEs on Complicated Domains

Stefan Sauter (University of Zurich)

The discretisation of boundary value problems on complicated domains cannot resolve all geometric details such as small holes or pores. The model problem of this paper consists of a triangulated polygonal domain with holes of a size of the mesh-width at most and mixed boundary conditions for the Poisson equation. Reliable and efficient a posteriori error

estimates are presented for a fully numerical discretisation with conforming piecewise affine finite elements. Emphasis is on technical difficulties with the numerical approximation of the domain and their influence on the constants in the reliability and efficiency estimates. This talk comprises joint work with Carsten Carstensen.

Mathematical Models of Fluids with Structure

Noel J. Walkington (Carnegie Mellon University, Pittsburgh)

Liquid crystals, fluids containing elastic particles (such as blood), and polymer fluids, all exhibit non-trivial macroscopic behavior due to interactions occuring on micro/mesoscopic scales. The derivation of rational models for these materials is a non-trivial task and typically results in formidable systems of partial differential equations; however, the mathematical structure of the underlying systems has much in common. Of these problems the most complete theory is for Ericksen's model of liquid crystal, and I will begin with a discussion of this theory and the corresponding numerical analysis. I will then consider fluids containing elastic particles and present a novel approach which eliminates the need to consider different coordinate systems for the particles (Lagrangian) and fluid (Eulerian). This naturally leads one to consider some fascinating models developed in the physics community which model polymer fluids and provide more refined models for liquid crystals. These latter ideas are not widely known in the mathematical community.
This is joint work with C. Liu (Pennsylvania State University, USA).

Numerics of the Cahn-Hilliard model

Ulrich Weikard (University of Bonn)

After introducing and motivating the Cahn–Hilliard model we present a fully discrete finite element approximation. We derive local a posteriori error estimates and show how to use them for mesh adaption.

Furthermore, we consider a fully discrete approximation scheme for the Cahn–Hilliard equation with elasticity

$$\begin{aligned} \frac{\partial \rho}{\partial t} &= \Delta\Big(\psi'(\rho) - \gamma\Delta\rho - \mathcal{S} : \bar{\mathcal{E}}'(\rho) + (\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho)) : \mathcal{C}'(\rho)(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho))\Big), \\ 0 &= \operatorname{div} \mathcal{S}, \\ \mathcal{S} &= \mathcal{C}(\rho)(\mathcal{E}(\mathbf{u}) - \bar{\mathcal{E}}(\rho)), \end{aligned}$$

where ψ is the homogeneous free energy, $\mathcal{S}$ the stress, $\mathcal{E}$ the strain and $\bar{\mathcal{E}}(\rho)$ denotes the stress free strain at concentration ρ. In this model the elasticity tensor $\mathcal{C}$ depends on the concentration ρ. Additionally anisotropic effects can be incorporated via an appropriate choice of $\mathcal{C}$. Numerical calculations with anisotropic, inhomogeneous elasticity yield results that closely resemble experimental data.
Joint work with H. Garcke and M. Rumpf.

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