Mathematisches Forschungsinstitut Oberwolfach

Tagungsbericht 17/99

Numerics of Microstructures

25.04.-01.05.1999

Organizers: Carsten Carstensen, Kiel
Wolfgang Hackbusch, Leipzig
Mitchell B. Luskin, Minneapolis

The Oberwolfach meeting of 25.04.-01.05.1999 on " Numerics of Microstructure" brought together the leading experts working on numerical methods for microstructure in a wide variety of physical systems. Microstructure is found in many physical systems as the small scale oscillations in a physical variable. For many of the physical systems discussed, the microstructure arises from the mixture of symmetry-related states on a fine scale to minimize energy. Microstructure and its numerical computation was discussed for the deformation gradient in martensitic crystals and the magnetization in ferromagnetic crystals. Microstructure was also discussed for plastic materials, porous media, composite materials, and elastic materials with fine scale cracks and inclusions. Among the methods discussed were finite element methods, relaxation methods, special multi-scale methods, and integral equations.

Abstracts of Plenary Lectures

Finite element analysis for a relaxed problem in micromagnetics

Carsten Carstensen

Starting from the classical minimisation problem for the modelling of micromagnetic bodies, the exchange energy is neglected and the remaining non-convex energy density is convexified following the works of Tartar, DeSimone and others. The relaxed problem is convex (and solutions exist) but not strictly convex (and so multiple solutions are possible). Even in cases where there exists a unique solution for the exact (relaxed) model, the natural discretisation fails and examples are presented with multiple discrete solutions and non-convergence of the magnetic field approximation. A nonconforming approach yields a unique discrete solution and sharp a priori error estimates (in the sense of an optimal bound). Numerical experience supports the choice of the penalisation parameter (to treat the convexified saturation condition) and effects that depend on the alignment of the mesh with the easy axis.

Carsten Carstensen, Mathematisches Seminar, Universität Kiel

On the formation of microstructures in problems with incompatible wells

Michel Chipot

For a function $\varphi : M_{2,2} \to \mathbb{R}^+$ vanishing on some wells we exhibit minimizing sequences of the problem

$$\inf_{v \in W_0^{(1,\infty)}(\Omega)} \int_\Omega \varphi(\nabla v(x))\, dx$$

and show their complexity.

Michel Chipot, University of Zurich

A Discontinuous Finite Element Method for laminated Microstructure

Matthias K. Gobbert

Numerical computations have been performed using conforming, nonconforming and discontinuous finite elements. Both classical methods suffer from suboptimal convergence rates (half order in the mesh parameter) and a strong dependence on the alignment between the numerical grid and the physical laminates. This talk presents a discontinuous finite element, for which an optimal convergence estimate for the energy has been shown (second order in the mesh parameter). Computational results demonstrate both the convergence rate and the independence from the mesh alignment.

Matthias K. Gobbert, Department of Mathematics and Statistics, University of Maryland, Baltimore County

---

On microstructures occurring in a model of finite–strain elastoplasticity involving a single slip-system

Klaus Hackl

We start by deriving a novel variational principle for a time–discretized model of the flow theory of elastoplasticity at finite strains. Within a single time–step we can thus formulate a minimization problem with respect to the total deformation and the update of the plastic deformation gradient. For a specific model involving a single slip–system the latter quantity can be eliminated. The resulting minimization problem with respect to the total deformation as single variable can be shown to be not rank–one–convex.

Finite element calculations indeed show the occurrence of layered microstructures . The results are, however, mesh–dependent. To overcome this effect a rank-one–convexification of the potential at hand is performed numerically using a gradient–line search–algorithm. The results obtained using the relaxed potential are more regular and essentially mesh–independent, although there are some hints at the presence of microstructures of higher order.

Klaus Hackl, Institute for Strength of Materials, Technical University of Graz.

Integral equation methods and numerical solutions for fracture mechanics problems

Johan Helsing

We discuss the conditioning of simple 2D-elliptic problems related to fracture mechanics. An example is an elastic plane with elastic inclusion and cracks. We argue that these problems are well-conditioned and that it should be positive to solve them rapidly and to high accuracy using stable algorithms. we sketch a six point plan for how this can be done. Key ingredients include the transformation of the PDE into a Fredholm integral equation of the second kind, and the use of fast multipole accelerated iterative solvers for systems of linear equations. A numerical example solves a fracture mechanics problem involving 10.000 randomly oriented cracks.

Johan Helsing, Solid Mechanics KTH, Stockholm

Multiscale Finite Element Computations for Flow and Transport in Strongly Heterogeneous Porous Media

Thomas Y. Hou

We introduce a multiscale finite element method for computing flow and transport in strongly heterogeneous porous media which contain many spatial scales.

The method is designed to effectly capture the large scale behavior of the solution without resolving all the small scale features. This is accomplished by constructing the multiscale finite elementbase functions that incorporate local microstructures of the differntial operator. Our method is applicable to general multiple-scale problems without restrictive assumption on scale separation and periodicity. Convergence of our method has been established in the case of periodic oscillatory structures. The rate of convergence is shown to be independent of the small scales of the solution. We demonstrate the accuracy and robustness of our method through extensive numerical experiments, which include the scale-up of two-phase flows with strongly shear random permeability, wave propagation through heterogeneous media, and convection enhanced diffusion. Steady condiction through fiber composites and flows through random media with normal and fractal porosity distributions will also be considered. Parallel implementation and performance of the method will be addressed.

Thomas Y. Hou, Applied Mathematics 217-50, California Institute of Technology, Pasadena, CA 91125, U.S.A.

A Geometrically Linear, Diffuse-Interface Approach to Microstructural Evolution in Martensite

Matthew G. Killough

Inspired by the experiments of Chu and James, we focus on the stress-induced transformation from one variant of martensite to another. We propose a geometrically linear multi-well elastic energy regularized by quadratic strain gradient terms and study the microstructural evolution using a relaxation law. This formulation greatly simplifies the task of developing an efficient numerical algorithm and allows us to compute long-time evolution of moderatly complicated microstructures.

We justify our unconventional choice of kinetics by computing it to two more traditional choices. On one hand, our approach is equivalent to a quasi-static kinetic law for the total (elastic + surface) energy. On the other, it approximates a sharp-interface, quasi-static approach with a particular anisotropic kinetic relation.

Finally we present some results of numerical experiments showing microstructural evolution which closely minimies the physical experiments.

Matthew G. Killough, School of Mathematics, University of Minnesota, U.S.A.

Numerical approximation of Young measures in relaxed problems in micromagnetics

Martin Kružík

The paper deals with two-dimensional computations of relaxed problems in micromagnetics for uniaxial materials. As the set of admissible magnetizations is not weakly closed we cannot proceed with the direct method when proving the existence of a minimum of an energy functional and some relaxation is needed. We use the relaxation utilizing Young measures. Computational results for various applied external magnetic fields and computed microstructures are shown. The convergence of solutions to approximative problems to a solution of the relaxed problem is established.

Martin Kružík, Institute of Information Theory and Automation, Academy of Sciences of the Czech Republic

---

On the Stability of Microstructure: The Tetragonal to Monoclinic Transformation

Mitchell B. Luskin

We give an analysis of the stability and uniqueness of the simply laminated microstructure for the tetragonal to monoclinic transformations. The energy density for the tetragonal to monoclinic transformation has four rotationally invariant wells. We show that the simply laminated microstructure is stable except for a class of special material parameters. In each case that the microstructure is stable we derive error estimates for the finite element approximation.

Mitchell B. Luskin (joint work with Pavel Belik), School of Mathematics, University of Minnesota, U.S.A.

Asymptotic analysis of laminar viscous flow over a porous bed

Nicolas Neuss, Willi Jäger, Andre Michelic

We consider laminar viscous channel flow over a porous bed containing periodically distributed pores of small size. We study the corresponding boundary layers and discuss their numerical approximation. A rigorous asymptotic expansion then yields Saffman's modification of the Beavers-Joseph interface law. Constants appearing in this law are computed from the solution of the boundary layer cell problem.

Nicolas Neuss, Universität Heidelberg
Willi Jäger, Universität Heidelberg
Andre Michelic, Univeristé Lyon.

Relaxation and microstructure with a length-scale

Petr Plecháč

The relaxed problem for two-phase elastic media is discussed. In the linearised- elasticity setting the relaxation is known explicitely (due to R. V. Kohn). The explicit quasiconvex envelope allows us to analyse approximation of certain macroscopic quantities. We present a posteriori error indicators and their application in design of an adaptive mesh refinement.

The relaxation can be seen as a "limit" over infinite number of scales. In many problems the scale is, however, fixed by regularising terms in the energy functional. We discuss a problem of optimal design for imperfectly bounded conductors to demonstrate that finite length-scale have to be taken into account. Numerical analysis of the resulting minimisation problem is presented.

Petr Plecháč, Mathematical Institute, University of Oxford

Direct Minimization in Micromagnetics

Andreas Prohl

During the talk, a conforming finite element method is discussed to minimize a bounded energy functional in micromagnetism (i.e., assembled from anisotropic (local) and stray-field (nonlocal)) energy. Well-known finite element analyses (Luskin, Ma '92) are built on constructing an admissible function on a numerical mesh that is aligned with the easy axis (uniaxial material).

In the present approach, general meshes are admitted for the error analysis. The results of convergence to real minimal energy are obtained using more sophisticated candidates showing branching structures in the vicinity of the boundary of the ferromagnet of the present mesh.

In the (more symmetric) cubic case, one can even obtain convergence statements that are superior to those for the uniaxial case. From the branching structures close to the boundary a graduate mesh strategy together with an adaptive concept is proposed to obtain improved results of convergence to the real minimal energy.

Andreas Prohl, Mathematisches Seminar, Universität Kiel

Numerical optimal design of stratified media.

Tomáš Roubíček

The optimal control of a linear elliptic equation with control acting as a coefficient matrix varying in a single direction only was considered. The problem may not have any solutions, so it must be suitable relaxed. Here, Young measures to describe stratified composites were used, optimality conditions were derived and a numerical scheme based on a piecewise constant approximation of Young measures was developed and analyzed, including rate-of-error estimates.

Tomáš Roubíček, Mathematical Institute, Charles University, Praha

---

A posteriori error estimation on complicated domains

Stefan Sauter

Composite finite elements allow coarse scale dicretizations of partial differential equations on complicated domains. The minimal number of unknowns is independent of the size and number of geometric details. In our talk we present a posteriori error estimators which are reliable also on the very coarse discretization levels. This results in highly adapted finite element spaces in the presence of, e.g. many holes or thin structures in the domain.

Stefan Sauter, Mathematisches Institut, Universität Leipzig

Generalized p-FEM for problems with periodic microstructure

Christoph Schwab

For problems with periodic, rapidly oscillating coefficients, we construct spectral FE-spaces that incorporate the local properties of the operator. We prove that exponential convergence can be achieved even for very rough (L^∞_{per}) coefficients, if the right hand side is analytic. Numerical results confirm the estimates. The method appears to be consistent of higher order in the scale parameter as well.

Christoph Schwab (joint work with A.M. Matache & I. Babuska), Seminar of Applied Mathematics ETHZ, Zurich

---

A New Class of Extremal Composites inspired by Topology Optimazation

Ole Sigmund

The paper presents a new class of two- and three-phase elastic composites with extremal bulk moduli. The new class of extremal materials constitutes an alternative to the three previously known classes namely finite-rank laminates, composites sphere assemblages and Vigdergauz microstrucures. Furthermore, some two-phase microstructures belonging to the new class have lower shear moduli than any previously known composite and some three-phase microstrucures belonging to the new class have higher bulk-moduli than any previously known composites. The new micro geometries are inspired by results from numerical topology optimization of microstructures.

Ole Sigmund, Department of Solid Mechanics, Technical University of Denmark, Lyngby

List of participants

NAME	e-mail adress
Carstensen, Carsten	cc@numerik.uni-kiel.de URL: http://www.numerik.uni-kiel.de/cc/
Chipot, Michel	chipot@amath.unizh.ch URL: http://www.math.unizh.ch/~chipot/
Gobbert, Matthias K.	gobbert@math.umbc.edu URL: http://www.math.umbc.edu/~gobbert
Hackbusch, Wolfgang	wh@mis.mpg.de URL: http://www.numerik.uni-kiel.de
Hackl, Klaus	hackl@euler.tu-graz.ac.at
Helsing, Johan	helsing@nada.kth.se URL: http://www.nada.kth.se/~helsing
Hou, Thomas Y.	hou@ama.caltech.edu URL: http://www.ama.caltech.edu/~hou
Killough, Matthew G.	killough@math.umn.edu URL: http://www.math.umn.edu/~killough
Kružík, Martin	kruzik@utia.cas.cz
Luskin, Mitchell B.	luskin@math.umn.edu URL: http://www.math.umn.edu/~luskin
Neuss, Nicolas	Nicolas.Neuss@iwr.uni-heidelberg.de URL: http://www.iwr.uni-heidelberg.de/~Nicolas.Neuss
Plecháč, Petr	plechac@math.udel.edu URL: http://www.math.udel.edu/~plechac
Prohl, Andreas	apr@numerik.uni-kiel.de URL: http://www.numerik.uni-kiel.de/~apr
Roubíček, Tomáš	roubicek@karlin.mff.cuni.cz URL: http://www.karlin.mff.cuni.cz/~roubicek
Sauter, Stefan	sas@mathematik.uni-leipzig.de URL: http://www.mathematik.uni-leipzig.de/numerik/homesa.html
Schwab, Christoph	schwab@sam.math.ethz.ch URL: http://www.sam.math.ethz.ch/~schwab
Sigmund, Ole	sigmund@fam.dtu.dk URL: http://www.fam.dtu.dk./html/os.html

Berichterstatter: A. Prohl

Tagungsteilnehmer

Prof.Dr. Carsten Carstensen
Mathematisches Seminar
Universität Kiel
Ludewig-Meyn-Str. 4

24118 Kiel

Prof.Dr. Michel Chipot
Institut für Angewandte Mathematik
Universität Zürich
Winterthurerstr. 190

CH-8057 Zürich

Prof.Dr. Matthias K. Gobbert
Dept. of Mathematics and Statistics
UMBC
1000 Hilltop circle

Baltimore , MD 21250
USA

Prof.Dr. Wolfgang Hackbusch
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26

04103 Leipzig

Dr. Klaus Hackl
Institut für Festigkeitslehre
Technische Universität
Kopernikusgasse 24

A-8010 Graz

Prof.Dr. Johan Helsing
Dept. of Solid Mechanics
Royal Institute of Technology

S-10044 Stockholm

Prof.Dr. Thomas Y. Hou
Applied Mathematics 217-50
California Institute of Technology

Pasadena , CA 91125
USA

Prof.Dr. Matthew G. Killough
School of Mathematics
University of Minnesota
127 Vincent Hall
206 Church Street S. E.

Minneapolis , MN 55455
USA

Prof.Dr. Martin Kruzik
Max-Planck-Institut für Mathematik
in den Naturwissenschaften
Inselstr. 22 - 26

04103 Leipzig

Prof.Dr. Mitchell B. Luskin
School of Mathematics
University of Minnesota
127 Vincent Hall
206 Church Street S. E.

Minneapolis , MN 55455
USA

Nicolas Neuss
Interdisziplinäres Zentrum
für Wissenschaftliches Rechnen
Universität Heidelberg
Im Neuenheimer Feld 368

69120 Heidelberg

Prof.Dr. Petr Plechac
Department of Mathematical Sciences
University of Delaware
501 Ewing Hall

Newark , DE 19716-2553
USA

Dr. Andreas Prohl
Mathematisches Seminar
Universität Kiel

24098 Kiel

Prof.Dr. Tomas Roubichek
Mathematical Institute
Charles University
Sokolovska 83

186 00 Praha 8
CZECH REPUBLIC

Prof.Dr. Stefan A. Sauter
Mathematik Departement
ETH Zürich
ETH-Zentrum
Rämistr. 101

CH-8092 Zürich

Prof.Dr. Christoph Schwab
Seminar für Angewandte Mathematik
ETH-Zentrum
Rämistr. 101

CH-8092 Zürich

Prof.Dr. Ole Sigmund
Department of Solid Mechanics
Building 404
Technical University of Denmark

DK-2800 Lyngby