Mathematisches Forschungsinstitut Oberwolfach

Report No. 33/2003

# Multiple Scale Systems-Modelling, Analysis and Numerics

July 27th – August 2nd, 2003

Organizers: Willi Jaeger (Heidelberg) jaeger@iwr.uni-heidelberg.de
Andro Mikelic (Lyon) Andro.Mikelic@univ-lyon1.fr
Christoph Schwab (Zuerich) schwab@math.ethz.ch

**1. Background** In recent years, applied mathematics has seen a spectacular development in the description of systems with multiple length scales. This was driven by the need to understand the impact of microscopic, even atomistic, phenomena on the macroscopic properties of systems that had been traditionally described by partial differential equations. As a consequence, the classical continuum-mechanics-based mathematical models in the sciences have been extended and coupled to incorporate atomistic effects.

The development is driven by the recent progress in micro- and nanotechnology, an increase in computing power which revealed shortcomings of the continuum-models on the one hand and by the emergence of new analytical tools to describe the scale-interaction in mathematical models; we mention as problems phase-transitions in solids, pattern formation in biology, kinetic descriptions of rarefied flows, chemically reacting flows; the precise modelling of biomaterials (bone and muscle-tissue) as well as lattice- materials in engineering. Classical mathematica homogenizations, while well-established, have been inadequate in many cases and have been substantially refined - we mention renormalization, $H$-measures, $\Gamma$-convergence. While these allow to treat successfully certain problem-classes with sufficient structure (e.g. ergodicity or periodicity) it has become clear that large and important problem classes are yet intractable; these are e.g. fractal domains and patterns, non-ergodic stochastic models, problems with multiple spatial and temporal scales that are not known a-priori or that change dynamically.

**2. The meeting.** The meeting brought together 42 researchers from Europe and overseas, from very diverse areas of mathematics as well as from applications areas.

An important factor was the high number of young researchers (11 **Check**) who contributed through short talks on their work as well as through often interaction with more senior speakers.

The scope of the talks was intentionally very broad: it ranged from pure analysis with with talks from the Calculus of Variations (such as the talks of Müller and Fonseca), to talks covering algorithmic and numerical analysis aspects of Multiscale Problems (talks of Carstensen, Weinan E, Griebel, Melenk, Neuss, Schweizer) to strongly applications oriented talks such as the one of Canic on multiscale problems in models of human arteries, or the talk by Paloka. These were complemented by presentations of recent results on classical homogenization theory, mainly from the Russian School, by e.g. Berlyand, Yurinski, but also from Neuss-Radu, for example.

**3. Problem Session.**

On the evening of Thursday, July 31, 2003, a problem session was held.

A number of open problems was presented. S. Müller presented new membrane models unknown before in the engineering and found as gamma-limits of thin nonlinear elastic structures. Then there was discussion about threshold parameters for non-linear problems e.g. Navier-Stokes leading to the ill-posed 2-pressures Euler (A.M., S. Luckhaus, B. Schweizer), then on stochastic homogenization, on blood flows and modelling of branching (W. Jaeger, E. Marusic-Paloka), problems in Calculus of Variations by G. Butazzo.

U. Mosco asserted that asymptotic limiting models should be embedded into hierarchies of models where the "higher order" members of such hierarchies should be derived by epi-convergence.

**4. List of participants.**

It follows the list of participants in the meeting in alphabetical order with the title of the talk, where applicable.

Ansini, Nadia (Roma)

Berlyand, Leonid (University Park)
"Network approximation for highly packed random composites"

Bornemann, Folkmar A. (München)
"Energy-level crossings in MD - is there a mathematical passage?"

Bouchitte, Guy (La Garde)
"Homogenization of second order energies on periodic thin structures"

Buttazzo, Giuseppe (Pisa)
"Optimization problems for mass transportation"

Canic, Suncica (Houston)
"Multiscale modeling in blood flow problems"

Capasso, Vincenzo (Milano (I))
"Coupling Stochastic Geometries and Heat Transfer in Crystallization Processes"

Carstensen, Carsten (Wien)
"Remarks on the numerical analysis of relaxed minimisation models
in three applications"

Cioranescu, Doina (Paris) "Periodic Unfolding Technique for Homogenization of Problems with Multiple Scales" (no abstract provided)

E, Weinan (Princeton)
"Multi-scale analysis of complex fluids, or multi-scale problems in material sciences"

Engquist, Björn (Los Angeles)
"Heterogeneous multiscale methods"

Fonseca, Irene (Pittsburgh)
"Asymptotic domain wall energy in micromagnetism"

Friedmann, Elfriede (Heidelberg)

Griebel, Michael (Bonn)
"Multiscale atomistic-continuum simulation of shape memory alloys"

Heinze, Steffen (Heidelberg)

“Front propagation in inhomogeneous media”

Heuser, Philip (Heidelberg)

Hoang, Viet Ha (Zürich)

Jäger, Willi (Heidelberg)

Lacharme, Severine (Villeurbanne)

Lenzinger, Michael (Heidelberg)

Luckhaus, Stephan (Leipzig)

Marusic-Paloka, Eduard (Zagreb)
“Mathematical modeling of an underground waste disposal site via homogenization (upscaling)”

Matache, Ana-Maria (Zürich)

Melenk, Markus (Leipzig)
“A two-scale regularity result for a homogenization problem with non-smooth fine scale geometry”

Michel, Eberhard (Heidelberg)

Mihailovici, Monika (Heidelberg)

Mikelic, Andro (Villeurbanne)

Mosco, Umberto (Roma)
“Fractal layers”

Moyne, Christian (Vandoeuvre les Nancy)
“Two-scale modeling of swelling clays”

Müller, Stefan (Leipzig)
“A hierarchy of plate models derived from nonlinear elasticity by Γ-convergence and folding patterns in thin films”

Murad, Marcio (Petropolis)
“A Dual Porosity Model for Electrical Charge Transport in Swelling Clays”

Neuss, Nicolas (Heidelberg)
“Fast numerical computation of constants in effective laws”

Neuss-Radu, Maria (Heidelberg)

Niethammer, Barbara (Bonn)
“On the influence of screening and correlations on phase separation”

Pastukhova, Svetlana (Moscow)
“Homogenization of Elasticity Problems on Thin Periodic Lattices of Critical Thickness”

Piatnitski, Andrey (Moscow)
Averaging of nonlinear random parabolic operators with large potential

Schwab, Christoph (Zürich)

Schweizer, Ben (Heidelberg)
“Homogenization of Fronts in Porous Media”

Svanstedt, Nils (Gothenburg)

"Two-scale compensated compactness"

Warnke, Rainer (Zürich)

Yurinsky, Vadim (Covilha)
"Asymptotics of the Principal Eigenvalue for the Stokes Operator in a Random Domain"

Zhikov, Vasily V. (Vladimir)
" On spectral gaps of periodic divergence form operators "

**5. Final Programme.**
Here we present the final programme of talks and events during the meeting.

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Monday July 28:

9h-9h15 Opening by Willi Jaeger (Heidelberg)

9h15 - 10h  Piatnitski Andrey (Narvik and Moscow) andrey@sci.lebedev.ru
: Averaging of nonlinear random parabolic operators with large potential

10h - 10h45 Capasso Vincenzo (Milano) capasso@mat.unimi.it
 : Coupling Stochastic Geometries and heat transfer in crystallization
 processes

10h45-11h30  Coffee Break

11h30-12h15 Engquist Bjoern  (Princeton) engquist@princeton.edu
: Heterogeneous multiscale methods

12h30-15h30 Lunch Break

15h15- 16h Schweizer Ben (Leipzig and Heidelberg)
ben.schweizer@iwr.uni-heidelberg.de
 : Homogenization of fronts in porous media

16h - 16h45 Yurinsky Vadim (Covilha) yurinsky@ubi.pt
: Asymptotics of the principal eigenvalue for the Stokes
operator in a random domain

16h45-17h Break

17h- 17h45 Marusic-Paloka Eduard (Zagreb) emarusic@cromath.math.hr
: Mathematical modeling of an underground waste disposal site
via homogenization (upscaling)
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18h30 Dinner

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Tuesday July 29:

9h-9h45 Berlyand Leonid (University Park) berlyand@math.psu.edu
: Network approximation for highly packed suspensions of solid particles. Stability and metastability.

9h45 - 10h30 Bornnemann Folkmar A. (Muenchen) bornemann@ma.tum.de
: Energy level crossings: is there a mathematical passage ?

10h30 - 11h Coffee Break

11h-11h45 Niethammer Barbara (Bonn) barbara@iam.uni-bonn.de
: On the influence of screening and correlations on phase separation.

11h45-12h30 Carstensen Carsten (Wien) Carsten.Carstensen@tuwien.ac.at
: Remarks on the numerical analysis of relaxed minimization models in 3D applications

12h30-15h30 Lunch Break

15h30- 16h15 Heinze Steffen (Leipzig) heinze@mis.mpg.de
: Convection enhanced diffusion and reaction

16h15 - 17h Neuss Nicolas (Heidelberg) Nicolas.Neuss@iwr.uni-heidelberg.de
: Fast numerical computation of constants in effective laws

17h-17h15 Break

17h15- 18h Melenk Markus (Leipzig) melenk@mis.mpg.de
: Two-scale regularity result of homogenization problems and two-scale finite element convergence theory

18h30 Dinner

20h-20h45 Canic Suncica (Houston) canic@math.uh.edu
: Multiscale modeling in blood flow problems.

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Wednesday July 30:

9h-9h45 Fonseca Irene (Pittsburgh) fonseca@cmu.edu
: Higher order variational problems

9h45 - 10h30 Mueller Stefan (Leipzig) sm@mis.mpg.de
: Multiscale following patterns in thin films and this rigorous derivation of plate theories

10h30 - 11h Coffee Break

11h-11h45 Cioranescu Doina (Paris) cioran@ann.jussieu.fr
: On the unfolding method. Application to Stokes problem.

11h45-12h30 Svanstedt Nils (Gothenburg) nilss@math.chalmers.se
: Two-scale compensated compactness

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Thursday July 31

9h-9h45 Mosco Umberto (Roma)umberto.mosco@uniroma1.it
: Fractal layers

9h45 - 10h30 Bouchitte Guy (Toulon) bouchitte@univ-tin.fr
: Homogenization of second order energies on periodic thin structures

10h30 - 11h Coffee Break

11h-11h45 E Weinan (Princeton) weinan@princeton.edu
: Multi-scale analysis of complex fluids,
or multi-scale problems in material sciences

11h45-12h30 Buttazzo Giuseppe (Pisa) buttazzo@dm.unipi.it
: Optimization problems for mass transportation

12h30-15h30 Lunch Break

15h30- 16h15 Pastukhova Svetlana (Vladimir) zhikov@vgpu.elcom.ru
: Homogenization of elasticity problems on thin periodic lattices
of critical thickness

16h15 - 17h Moyne Christian (Nancy) Christian.Moyne@ensem.inpl-nancy.fr
: Two-scale modeling of swelling clays

17h-17h15 Break

17h15- 18h Murad Marcio (Petropolis) murad@lncc.br
: A dual porosity model for electrical charge transport in
swelling clays

18h30 Dinner

20h-20h45 Problem Session

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Friday August 1:

9h-9h45 Neuss-Radu Maria (Heidelberg) Maria.Neuss-Radu@iwr.uni-heidelberg.de
: Effective laws for curved oscillating boundaries

9h45 - 10h30 Luckhaus Stephan (Leipzig) luckhaus@mis.mpg.de
: Many scales in a model of " tumor development "

10h30 - 11h Coffee Break

11h-11h45 Griebel Michael (Bonn) griebel@iam.uni-bonn.de
: Multiscale atomistic-continuum simulation of shape memory alloys

11h45-12h30 Zhikov Vasily V. (Vladimir) zhikov@vgpu.elcom.ru
: On spectral gaps of periodic divergence form operators

CLOSURE

# Abstracts

### Network approximation for highly packed suspensions of solved particles, stability and metastability

Leonid Berlyand, Penn State University, USA
(joint work with L. Borcea and A. Panchenko)

We present a new approach for calculation of effective properties of high contrast in highly packed composites and provide its rigorous mathematical justification. The main idea of this approach is the reduction of the original continuum problem, which is described by PDE with rough coefficients, to a discrete problem for a random network.

We introduce the interparticle distance parameter $\delta$ for irregular (non-periodic) distribution of particles and show asymptotic equivalence between the continuum and the discrete problems in the limit $\delta \to 0$. The latter includes an analytical explicit error estimate.

Our method explains why theoretical results for effective viscosity of such suspensions did not agree with recent numerical and experimental data. The key observation is that local analysis may be misleading and global analysis is necessary.

### Energy-level crossings in MD - is there a mathematical passage?

Folkmar Bornemann, TU München, Germany

We consider time-dependent Born-Oppenheimer approximation and the Car-Parrinello method at energy, level crossings. For Car-Parrinello it is shown that there are problems at closing gaps or actual crossings. At a crossing we show that even in an averaged sense there is no reasonable convergence to the limit solution. Based on rigorous error estimates we propose an algorithm to control the fictitious electronic mass in the closing gap situation. For Born-Oppenheimer the crossing introduces a further scale of $O(\varepsilon^{\frac{1}{2}})$. We review recent results of Lasser and Teufel about a rigorous surface hopping algorithm.

### Optimization problems for mass transportation

Giuseppe Buttazzo, University of Pisa, Italy

Mass transportation problems deal with a metric space $(X, d)$ and two probability measures $f^+$ and $f^-$ on $X$. The cost functional

$$F(d) = \inf \left\{ \int\int_{X \times X} d(x,y)\, d\gamma(x,y) : \ \gamma \text{ has marginals } f^+ \text{ and } f^- \right\}$$

can be then defined, and its value depends on the distance $d$ we considered on $X$.

We give a model for the description of an urban transportation network and we consider the related optimization problem which consists in finding the design of the network which has the best transportation performances.

## Effective equations modelling the dynamics of large and small compliant arteries

Suncica Canic, University of Houston, USA
(joint work with A. Mikelić)

In this talk a comprehensive strategy of the fluid-structure interaction between the blood flow and the vessel wall was presented. The vessel walls are modelled by the Navier equations for the linearly elastic curved membrane and the flow of blood is assumed to satisfy the Navier-Stokes equations for incompressible viscous fluid in large arteries, and the Stokes equation in small arteries. Together with Andro Mikelić, University Claude Bernard, Lyon 1, France, a systematic, rigorous asymptotic analysis was presented to obtain the resulting, effective, one-dimensional equations. They are hyperbolic PDEs with dispersion (in large arteries) given in torus of the cross-sectional area of the vessel and the averaged flow (momentum). The resulting effective equations in small arteries are given in torus of the pressure. They are linear, parabolic, $4^{\text{th}}$ order PDEs corresponding to a set of Bio type viscoelastic equations for the effective pressure and true effective displacements.

Numerical simulations showing the difference between linear and nonlinear coupling between the fluid and the vessel wall were shown for the data corresponding to a healthy human abdominal aorta. Movies showing the dynamics of a "stented" artery were presented. They show high deformations near the anchoring sites of the "stent" indicating large stresses and strains of the vascular tissue.

## Coupling stochastic geometries and heat transfer in crystallization processes

Vincenzo Capasso, MIRIAM University of Milano, Italy

A mathematical model for crystallization of a class of materials (including polymers) is presented. it is based on a necleation-and-growth stochastic process strongly coupled with heat transfer; the kinetic parameters of nucleation and growth depend on the underlying temperature field; on the other hand the parameters and latent heat component in the evolution equation for temperature depend on the stochastic geometry of the crystalline phase. The crystallization process induces a stochastic tessellation of space whose morphology may be characterised in terms of the volume densities of interfaces at all relevant Hausdorff dimensions.

An optimal control problem is raised in industrial applications, based on existing relations morphology/mechanical properties of the solidified material. The controlling quantity is the applied extremal cooling temperature profile at the boundary.

An extension of the Kolmogorov-Arrami-Evans crystallization theory to deterministic space-time dependent kinetic parameters is provided, based on the concept of hazard function of the stochastic geometric crystallization process. Unfortunately due to the coupling, temperature induces stochasticity on the kinetic parameters. A double scale analysis leads to an hybrid model in which the evolution equation for temperature is homogenised at the larger scale to a deterministic one, leaving the geometric process stochastic at the lower scale, thus obtaining an hybrid model that now is treatable within the above quoted extended K-A-E theory.

The optimal control problem is now explored for the hybrid model.

Reference: V. Capasso ed., Mathematical Modelling for Polymer Processing. Math. in Industry, Vol. 2, Springer-Verlag, Heidelberg, 2003.

## Remarks on the numerical analysis of relaxed minimisation models in three applications

Carsten Carstensen, UT Vienna, Austria

The three applications considered for nonconvex minimisation problems model phase transitions, optimal design tasks, and micromagnetics. Since (quasi-) convexity is essentially equivalent to such weak lower semicontinuity, typically, the minimum in such nonconvex minimisation problems it **not** attained: Infimising sequences develop enforced oscillations of an arbitrarily time length scale and converge generalised solution. The approximation of this effective approximation is the task of a numerical simulation. In the direct approach to computational microstructures, the finite element solutions develop oscillations which are quite difficult to compute. In the three examples at hand, relaxation theory provides the effective, macroscopic models which are convex but not strictly or even uniformly convex. Then some a-priori and a-posteriori error control is available but there is a reliability efficiency gap and strong convergence in energy norms is under debate when stabilisation techniques are employed.

## Higher order variational problems

Irene Fonseca, Carnegie Mellon University, Pittsburgh, USA

Several problems in applied analysis motivated by questions in materials science, physics, computer vision, and other areas of engineering may be treated as higher order variational problems. Their study often requires state-of-the-art techniques, new ideas, and the introductions of innovative tests in partial differential equations, geometric measure theory, and the calculus of variations.

In this talk we show how some of these questions may be reduced to the study of well undenoted first order problems. In particular, a recent result obtained in collaboration with G. Dal Maso, G. Leoni and M. Morini generalizes a precisely obtained result by S. Müller and V. Šterák to assert that, under relatively mild assumptions, a 2-quasiconvex with superlinear growth at infinity may be extended to non-symmetric matrices on a "standard" 1-quasiconvex functions with the same growth.

Applications within the realm of phase transitions, of elasto-plastic materials, micromagnetism, and thin films are addressed.

## Multiscale atomistic-continuum simulation of shape memory alloys

Michael Griebel, Universität Bonn, Germany

Materials often show complex behaviour which needs to be resolved on different length scales. For example, certain microscopic effects can be described on an atomistic level using molecular dynamics, whereas macroscopic effects can be modelled on the continuum mechanical level. However, a direct numerical treatment of the coarser scale is usually not possible due to computational limits. To this end, advanced analytical and numerical techniques are needed to bridge the gap between the different scales. Here, we discuss the transition from the atomistic to the continuum mechanical level using techniques from statistical mechanics and multiscale analysis, where both scales are combined into one model simultaneously. We consider the example of crystalline microstructure in shape memory alloys to demonstrate our approach and show the results of various numerical experiments. This is joint work with Marcel Arndt (Bonn).

### Convection enhanced diffusion and reaction

Steffen Heinze, Max-Planck Institute, Leipzig, Germany

In the first part we consider a convection diffusion equation with an incompressible, periodic cellular flow field: $\partial_t u = \varepsilon \Delta u + b \cdot \nabla u$. After homogenization we provide explicit upper and lower bounds for the effective diffusivity in dependence of the viscosity $\varepsilon$. All estimates have the convect scaling for small $\xi$. The upper estimate also answers an open problem of residual diffusion, posed by Kozlov: For a $C^{\alpha}$-stream function there is no residual diffusion in contrast to the case of a discontinuous stream function. In the second part a nonlinear reaction of KPP type is added to the equation. The large time asymptotics is governed by travelling waves. For shear flows explicit bounds for their speed are derived, showing the correct scaling of the speed, especially in the large Pectet number limit. For cellular flows the expected scaling could be shown in the homogenized regime.

### Many scales in a model for "tumour development"

Stephan Luckhaus, MPI Leipzig, Germany
(joint work with L. Triolo)

Starting point is a lattice model for two populations modelling the competition between normal and malignant cells. We concentrate on just one difference-lateral contact inhibition, lacking in malignant cells, and the higher fertility of malignant cells.

The process has 5 independent parts:

- fast independent random walk of the malignant cells
- slower random motion of normal cells to empty neighbouring sites
- birth process for malignant cells
- birth process with the same rate for normal cells - if neighbouring sites are empty
- a death process for both types of cells with a rate depending on the occupation number of the site.

In the thermodynamic limit - still formal without an additional scaling - one gets a reaction-diffusion system. This always has a stable stationary point with no normal cells - mirroring their conditional and therefore higher birth rate. But if the death rate at occupation number two is sufficiently larger than the one of occupation number one, a second stable point appears with only normal cells surviving. This is due only to the fact that one evaluates the expected death rate correctly with respect to Poisson measure. The conclusion is first that the local invariant measure is crucially determining the behaviour - a mean field approach could give the wrong result - and second that enhancing the death rate for normal and malignant cells indiscriminately improve the survival chance for the normal cells.

### Modeling of an underground waste disposal site by upscaling

Eduard Marusic-Paloka, University of Zagreb, Croatia

The goal of this work is to give an accurate model describing the global behaviour of an underground waste repository array, made of a high number of units, since the units start to leak. A detailed description of such a model is given in complex exercise, and we use it as a shorting point for our analysis. The purpose of such a global model is to be used for simulations necessary for safety assessments.

We use homogenization and the boundary layer techniques to compute the zero order and the first order approximation of the original solution. We give the error estimate for our expansion as well as some simulations based on it.

## Two-scaled regularity for a homogenization problem with non-smooth fine scale geometry

Markus Melenk, MPI, Leipzig, Germany
(joint work with A.-M. Matache)

Elliptic problems on two-dimensional, infinite periodic (period $\varepsilon$) structures are analyzed, and two-scale regularity results for the solution are given. The emphasis of the analysis is placed on the case when the periodic structure, or, more generally, piecewise analytic, cavities, and the coefficients are (piecewise) analytic.

The solution $u^\epsilon$ enjoys scale separation properties, i.e., in terms of the right-hand side if it is given by

$$u^\varepsilon(x) = \int_{\mathbb{R}^2} \widehat{f}(t)\, e^{it\cdot x}\, \phi(\frac{x}{\varepsilon}, \varepsilon, t) dt\,,$$

where $\phi$ is the solution of an appropriate unit cell problem The regularity properties of $\phi$ are analysed in detail in dependence on the critical parameters $\varepsilon$, the wave vector $t$, and the differentiation order. Since the boundary of the cavities is not smooth, the solution exhibits corner regularities, which are accounted for by means of appropriate weighted Sobolev spaces.

The regularity results are derived with a view to an application in numerical methods such as the generalized FEM and the two-scale FEM of Matache & Schwab. In particular, our regularity results provide appropriate mesh design principles for the discretization of the unit cell in the two-scale FEM.

## Fractal layers

U. Mosco, University of Rome, Italy

Our reference problem is of the following type:

$Q_1$

$S$ $Q_2$

$$-\Delta u = f \quad Q_1 \cup Q_2 \quad u_i = u|_{Q_1} \quad i = 1, 2$$

$$\begin{cases} \dfrac{\partial u_1}{\partial \nu_1} + \dfrac{\partial u_2}{\partial \nu_2} = -\Delta_S\, u \text{ on } S \\ u_1 = u_2 \quad \text{on } S \end{cases}$$

fig-mosco.eps
235 × 31 mm

$$u = 0 \quad \partial(Q_1 \cup Q_2) \;\; u = 0 \;\; \partial S$$

2nd order transmission condition of this type were built by Ventsel (59), Couron-Meyer (71) in hydraulic fractioning, as highly conductive thin layers. Recently, M.R. Lancia and M.R. Lancia-M.A. Vivaldi, 2002-2003, considered model examples of **fractal** layers $S$. The broader perspective of this research, loosely speeding, consists in investigating: 1) interplay of Euclidean and fractal traces and Laplacians, 2) bvp with **small volume** and **big boundary**, 3) effective **Hölder matrices** to obtain metric scalings which have fractal geometry.

## A hierarchy of plate models derived from nonlinear elasticity by Γ-convergence and folding patterns in thin films

Stefan Müller, MPI, Leipzig, Germany
(joint work with G. Friesecke, R.D. Jones, H. Ben Belgacen, S. Conti and A. De Simone)

In the first part of the talk, which is joint work with G. Friesecke and R.D. Jones, we derive a hierarchy of plate models from three dimensional nonlinear elasticity by Γ-convergence. What distinguishes the different hint models is the scaling of the elastic energy per unit volume ($\sim \ell i^{\beta}$) in terms of the thickness $h$. This is in turn related to the scaling of the applied force $\sim h^{\alpha}$. In particular the widely popular FVK (Föppl, von-Karman) theory whose traditional derivation has not some severe criticism appears as a Gamma hint for $\alpha = 3$, leading to $\beta = 4$. In the second part of the talk (joint with H. Ben Belgacen, S. Conti and A. De Simone) I discuss complex folding patterns in thin films and derive the optimal energy scaling ($\beta = 1$) for this case.

## A dual porosity model for electric charge transport in expansing clays

Márcio Murad, LNCC, Brazil

In this talk we proposed a double porosity formulation to describe contaminant transport in expansive clays. The model is based on a three-scale approach. At the microscale the elasticity solution which contains completely dissociated ions $Na^{+}$ and $Cl^{-}$ or homogeneous with the elastic behaviour of the clay particle. That led to a Darcy-scale type model, a modified form of the Darcy law is derived continued with a modified form of Terraghi, decomposition and also modified convection-diffusion equation governing the movement of the ions.

By homogenizing the two-scale model with the hulk fluid in the macro-pores we obtained a dual porosity model wherein the clay clusters act as sources and scales of mass to the hulk phase vector in the macro-pores.

A quasi-strategy assumption is postulated and a retardation appears in the homogenized model which governs the adsorption/desorption of the chemical by the clay clusters. The three scale setting establishes a correlation between their parameter and the macroscale electric potential which satisfies a Poisson-Boltzman type equation.

## Effective laws for curved oscillating boundaries

Maria Neuss-Radu, University of Heidelberg, Germany
(joint work with N. Neuss and A. Mikelić)

We derive an effective boundary condition for oscillations superimposed on curved boundaries in the case of the Laplace equation. We prove on $O(\varepsilon^{\frac{3}{2}})$ error estimate with respect to the energy norm for the difference between the solution of the effective equation and the exact solution.

## Fast computation of effective coefficients

Nicolas Neuss, University of Heidelberg, Germany

In natural and engineering sciences, people are often interested in determining effective parameters. In this talk, we consider the calculation of such parameters in the case of media with periodic microstructure. The essential part of such calculations is the numerical solution of a cell problem which is defined either on the unit cube or on a semi-infinite boundary cell. The solution to this cell problem requires both mesh-adaptivity and the use of high-order finite elements. Additionally, blending techniques have to be used for approximating smooth boundaries and interfaces.

Multigrid is used for solving the arising linear systems. A special ingredient is the smoothing with an overlapping vertex-centred block Gauss-Seidel smoother which is shown to be robust with respect to the discretization order both theoretically and practically. Using this method we can compute effective constants very fast and with high precision which is demonstrated for several applications. For this purpose, we used the PDE toolbox FEMLISP which is written completely in the A1 language Common Lisp. Essential advantages compared with traditional approaches using Fortran, C, or C++ are the interactive environment, automatic memory management, dynamic typing, compilation at runtime, and dynamic object-oriented programming.

## On the effect of screening and correlations in phase transitions

Barbara Niethammer, University of Bonn, Germany
(joint work with A. Höing and F. Otto)

The last stage of a first order phase transition is characterized by coarsening of the phase distribution. We consider the regime when one phase has small volume fraction and consists of many small spherical particles. In this regime the classical theory by Lifshitz, Slyozov and Wagner (LSW) gives a nonlocal transport equation for the particle size distribution. Predictions based on this theory do however not agree with the experiment. In this talk we present a new method to derive first order corrections to the LSW-theory. In particular, we also allow for pair correlations between particles.

The main idea in the derivation is to relate the full system of particles to a system where a finite number of the particles has been removed. With this strategy we separate screening from correlation effects which allows for efficient calculation of conditional expectations.

Using a cluster expansion for the $N$-particle distribution we then can close the system on the level of the two-particle distribution.

## Averaging of nonlinear random parabolic operators with large potential

A. Piatnitski, University of Narvik and Moscow State University

We study a homogenization problem for a parabolic reaction diffusion type equation with large nonlinear potential, under the assumption that the spatial microstructure is periodic and that all the characteristics of this microstructure are stationary rapidly oscillating random processes. In particular, we can consider a model problem with finite-dimensional stationary driving process. If the processes involved possess sufficiently good mixing properties, the following homogenization result holds: a solution of the original reaction-diffusion equation converges in law in the energy functional space, to a solution of effective stochastic partial differential equation. The latter equation has a unique solution and thus defines the limit measure uniquely.

## Motion of fronts in porous media

Ben Schweizer, University of Heidelberg, Germany

We study the behavior of two immiscible fluids in a porous medium, in particular the motion of the front between the two fluids. We start from a microscopic model in which the single pore is resolved and the front consists of pieces of fluid-fluid interfaces and pieces of fluid-solid interfaces. Averages equations are derived for the instationary equation. This is done on a meso-scale on which the free boundary is still resolved.

The analysis shows that stationary models can not capture the effects and that periodic homogenization suggests averaged equations that are unphysical. In fact the periodic solution is a degenerate case and in the stochastic setting we find that the limiting pressure satisfies the physical equations almost surely.

## Twoscale compensated compactness

Nils Svanstedt, Chalmers University, Gothenburg, Sweden
(joint work with B. Birnir and N. Wellander)

We combine Nguetsengs two-scale convergence with the compensated compactness by Murat and Tartar. The main result is that we can pass to the two-scales limit for quadratic forms. This has many nice applications in the homogenization of equations in fluid dynamics, electromagnetics or equations of acoustics.

## Asymptotics of the principal eigenvalue for the Stokes operator in a random domain

Vadim Yurinsky, Universidade da Beira Interior, Covilha, Portugal

The talk is dedicated to the study of large volume asymptotic behavior of the principal eigenvalue of the Stokes operator acting on solenoidal vector valued functions over a random domain modelling the pore space in a cubic sample of porous material with disordered structure. The operator is considered under the zero Dirichlet condition on the boundary of the domain. The principal eigenvalue is shown to converge in probability to a non-random limit under appropriate normalization.

The approach used to establish deterministic behaviour of the principal eigenvalue is through an auxiliary problem where the random domain is substituted by a scaled random potential. The technique is based on the analysis of feasible values of pertinent Rayleigh rations for individual test functions (which was suggested in [1]). The characterization of the limit follows that of the author's subsequent paper [2].

[1] Merkl F., Wüthrich M.: Infinite volume asymptotics of the ground state energy in a scaled Poissonian potential. Ann. Inst. H. Poincaré, Probability and Statistics, 2002, vol. 38, No. 3, 253-284.
[2] Yurinsky V.: Localization of spectrum bottom of the Laplacian in the presence of scaled potential. Preprint: Centro de Matem. UB, Dept. Matem., Pré-preblicaşao, No. 3, Covilha, Portugal, 2002.

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