Minisymposium 8

Homogenisierung und Anwendungen

Leiterin des Symposiums:

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Die Homogenisierung ist eine Methode aus dem Bereich der asymptotischen Analysis welche erfolgreich bei der Untersuchung von Mehrskalenproblemen und den dabei auftretenden Skalenübergängen eingesetzt werden kann. Dabei handelt es sich um Prozesse, welche durch partielle Differentialgleichungen beschrieben werden können.

Die in diesem Zusammenhang auftretenden Fragestellungen sind:

- Kann man ein komplexes mikroskopisches Problem durch ein numerisch behandelbares, makroskopisches approximieren? Wie groß ist der dabei entstehende Fehler?
- Können vorhandene phänomenologisch hergeleitete, makroskopische Gesetze validiert werden, indem sie aus mikroskopischen Gesetzen mittels einer asymptotischen Analyse hergeleitet werden? Dabei kann die unterliegende mikroskopische Struktur periodischer oder stochastischer Natur sein.

Im Rahmen des Minisymposiums befassen wir uns mit Modellen, welche physikalische und chemische Prozesse in porösen Medien, biologischen Geweben, Verbundwerkstoffen und Netzwerken beschreiben.

Donnerstag, 21. September

Hörsaal 311 AVZ I, Endenicher Allee 11-13

15:00 – 15:50 **Andro Mikelić** *(Lyon)*

Rigorous upscaling of the reactive flow through a pore, under dominant Peclet and Damkohler numbers

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16:00 – 16:50 **Ben Schweizer** *(Basel)*

Averaging of flows with capillary hysteresis in stochastic porous media

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17:00 – 17:25 **Michael Lenzinger** *(Basel)*

Viscous fluid flow in bifurcating pipes

17:30 – 17:55 **Kasten Matthies** *(Bath)*

Exponential homogenization of periodic linear problems

Freitag, 22. September

Hörsaal 311 AVZ I, Endenicher Allee 11-13

15:00 – 15:25 **Dirk Hartmann** *(Heidelberg)*

From Discrete to Continuum Models in Mechanobiology

15:30 – 15:55 **Nicolas Neuss** *(Kiel)*

Multi-scale simulation of diffusion and absorption in chloroplasts

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16:00 – 16:25 **Mariya Ptashnyk** *(Heidelberg)*

Derivation of a macroscopic receptor-based model using homogenization techniques

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16:30 – 16:55 **Christof Eck** *(Erlangen)*

Homogenization for Phase Transitions with Microstructures

17:00 – 17:25 **Julia Orlik** *(Kaiserslautern)*

Homogenization of Strength, Fatigue and Creep Durability of Composites with Near Periodic Structure

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17:30 – 17:55 **Malte Peter** *(Bremen)*
Homogenisation of chemical degradation mechanisms inducing the evolution of the microstructure of the porous media

Vortragsauszüge

Andro Mikelić *(Lyon)*
Rigorous upscaling of the reactive flow through a pore, under dominant Peclet and Damkohler numbers

In this talk we present a rigorous derivation of the effective model for enhanced diffusion through a narrow and long 2D pore. The analysis uses a singular perturbation technique. Starting point is a local pore scale model describing the transport by convection and diffusion of a reactive solute. The solute particles undergo a first order reaction at the pore surface. The transport and reaction parameters are such that we have large, dominant Peclet and Damkohler numbers with respect to the ratio of characteristic transversal and longitudinal lengths (the small parameter epsilon). We give a rigorous mathematical justification of the effective behaviour for small epsilon. Error estimates are presented in the energy norm as well as in L-infinity and L-1 norms of the space variable. They guarantee the validity of the upscaled model. As a special case, we recover the well-known Taylor dispersion formula. It is important to note presence of both chemical reactions and dispersion effects in the upscaled coefficients. Under dominant Peclet and Damkohler numbers, hydrodynamics and chemistry effects are strongly coupled.

Ben Schweizer *(Basel)*
Averaging of flows with capillary hysteresis in stochastic porous media

The fluid in an unsaturated porous medium is described by Darcy's law. Conservation of mass provides an evolution equation that couples the pressure p and the saturation u. A second relation between p and u is determined by the effects of capillarity. In general, the capillary pressure is a set-valued map and the second relation is of the form $p \in p_c(u, \partial_t u)$. The multi-valued function p_c leads to hysteresis effects of play-type.

We construct weak and strong solutions to the hysteresis system and homogenize it for random distributions of the physical parameters. In the effective equations a new variable with the units of a pressure appears. This new variable encodes the history of the process. The averaged equations have irreversible scanning curves and reflect the properties of the physical system.

Michael Lenzinger *(Basel)*
Viscous fluid flow in bifurcating pipes

We consider the flow of a viscous Newtonian fluid in a bifurcation of thin three-dimensional pipes with a diameter-to-length ratio of order $O(\epsilon)$. The model is based on the steady-state Navier-Stokes equations with pressure conditions on the outflow boundaries. Our aim is to construct an asymptotic expansion in powers of the diameter ϵ and a Reynolds number Re_ϵ, representing the assumption of small data. This approximation is based on Poiseuille flow in the pipes which is matched to the solution of a local Stokes problem in the junction. In this way we are able to include the influence of the bifurcation geometry on the fluid flow. We show that the solution of the junction problem decays exponentially to Poiseuille flow in the pipes and derive error estimates in powers of ϵ and Re_ϵ. The obtained results generalize and improve the existing ones in literature. In particular, our results show that Kirchhoff's law of the balancing fluxes has to be corrected in $O(\epsilon)$ in order to obtain an adequate error estimate for the gradient of velocity.

Karsten Matthies *(Bath)*
Exponential homogenization of periodic linear problems

The homogenisation of a divergence type second order uniformly elliptic operator is considered with arbitrary L^∞ rapidly oscillating periodic coefficients, either with periodic boundary conditions or in the whole space. We show that if the right-hand side is analytic then by optimally truncating the full two-scale asymptotic expansion for the solution one obtains an approximation with an exponentially small error in the period of the rapid oscillation. The optimality of the exponential error bound is established for a one-dimensional example by giving the analogous lower bound.

Dirk Hartmann *(Heidelberg)*
From Discrete to Continuum Models in Mechanobiology

In the last years, mechanobiology has drawn a lot of attention in the physical sciences from an experimental and theoretical viewpoint. Systems are investigated on different scales ranging from single molecules up to whole organisms.

One central problem in mechanobiology is the derivation of appropriate constitutive relations for continuous models, which should account for such different effects as growth in cell cultures or active contraction of polymer-fibres in migrating cells. Many systems can be described relative easily with discrete models on a microscopic scale, e.g. single cells in cell cultures or polymer fibres in cells. Whereas continuous macroscopic descriptions are usually less straight forward.

As constitutive relations are usually given in terms of free energies, Γ-convergence is the ideal framework for rigorously bridging the gap between discrete microscopic and continuous macroscopic models. For simple cases also homogenisation formulas can be applied, which allow an explicit calculation of the involved stress tensors. As examples, the mechanics of growing cell cultures and actively moving cells (Keratocytes) will be discussed.

Nicolas Neuss *(Kiel)*
Multi-scale simulation of diffusion and absorption in chloroplasts

We construct a microscopic model for diffusion of proteins in the interior of chloroplasts which can be considered as a complex heterogeneous medium. Under the assumption of periodic heterogeneities, we derive a homogenised model for this process and prove estimates of the approximation error. We then verify the validity of the model numerically, and see that it is a good approximation even for non-periodic settings. Finally, we discuss the possibility of using the approximation for the construction of multiscale preconditioners.

Mariya Ptashnyk *(Heidelberg)*
Derivation of a macroscopic receptor-based model using homogenization techniques

The aim of this work is to derive a macroscopic model describing receptor-ligand binding from the microscopic description using the methods of asymptotic analysis. We study the problem of diffusive transport of biomolecules in the intercellular space, modeled as porous medium, and of their binding to the receptors located on the surface membranes of the cells. Cells are distributed periodically in a bounded domain. To describe this process we introduce a reaction-diffusion equation coupled with nonlinear ordinary differential equations on the boundary (on the cells surface). The existence and uniqueness of the solution of this problem is proved. We consider the limit, when the number of cells tends to infinity and at the same time their size tends to zero, while the volume fraction of the cells remains fixed. Using the two-scale convergence, we show that the sequence of solutions of the original problem converges to the solution of the so called macroscopic problem. To show the convergence of the nonlinear terms on the surfaces we use the periodic modulation (unfolding method).

Christof Eck *(Erlangen)*
Homogenization for Phase Transitions with Microstructures

Many phase transition processes exhibit microstructures of various types, important examples are dendritic and eutectic microstructures in the solidification of metallic alloys or microstructures in epitaxial growth processes of semiconductors. These microstructures are not given a priori, their computation is part of the solution process for the problems. Homogenization of such processes therefore does not lead to a purely macroscopic model, but to a two- or multiscale model that combines different models for the different relevant length scales. The derivation and analysis of such models is described for applications in solidification and epitaxial growth. The models are justified by an estimate for the model error. The numerical implementation of the models is briefly discussed and examples of numerical simulations are presented.

Julia Orlik *(Kaiserslautern)*

Homogenization of Strength, Fatigue and Creep Durability of Composites with Near Periodic Structure

The composite macro-strength and -durability is estimated using the approximation to the micro-stress field, known from the asymptotic theory of homogenization, and presented in terms of a non-local strength and durability condition. The macro-strength and -durability functional over the homogenized stress-field is determined by micro-geometry, elastic and strength properties of the periodicity cell. The uniform in time convergence of the micro- to the macro-strength and -durability condition is also proved based on the two-scale convergence of the micro-stresses to their first approximation. The approach is applicable to the durability description at fatigue, creep, impact loading and their combination.

Reference:

J. Orlik, Homogenization of strength, fatigue and creep durability of composites with near periodic structure, Mathematical Models and Methods in Applied Sciences, Vol. 15, No. 9(15), pp. 1329-1347, 2005.

Malte Peter *(Bremen)*

Homogenisation of chemical degradation mechanisms inducing the evolution of the microstructure of the porous media

Chemical degradation mechanisms of porous materials often induce a change of the pore geometry. A typical situation is when the reaction products take up more volume than the reactants. This effect cannot be captured by the standard periodic homogenisation method due to the local evolution of the microscopic domain. Using elements of two-scale convergence and periodic unfolding, a mathematically rigorous approach is suggested which allows the treatment of such problems. In particular, it makes use of a transformation to a stationary (periodic) reference domain on which the homogenisation can be performed. A physical interpretation also allows the direct modelling of the transformed problem. This is performed for the particular problem of concrete carbonation. It is shown that the resulting system of coupled semi-linear and quasi-linear parabolic pdes is well-posed and a-priori estimates are obtained allowing its homogenisation.