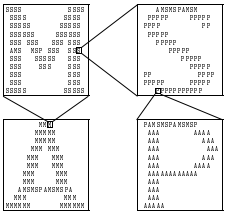
DFG Priority Programm

Analysis, Modeling and Simulation of Multiscale Problems



DFG-Forschungszentrum MATHEON
Mathematik für Schlüsseltechnologien

Leibniz Gemeinschaft

WIAS

Workshop on

Multiscale Problems in Three Applications

WIAS, Berlin

May 29 – June 01, 2007

Edited by

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Contents

General Information **2**

Programme **3**

Abstracts **6**

Thomas Böhme 6
Clemens Guhlke 7
Maren Hantke 8
Oliver Kastner 9
Christiane Kraus 10
Alexander Mielke 11
Alain Miranville 12
Luca Mugnai 13
Margarita Naldzhieva 14
Carsten Patz 15
Christian Rohde 16
Philip Rosenau 17
Matthias Röger 18
Björn Stinner 19
Anna Vainchtein 20
Juan Velazquez 21
Barbara Wagner 22
Jonathan Wattis 23

List of Participants **24**

General Information

Workshop on

Multiscale Problems in Three Applications

- **Sponsored by:**

  Weierstraß-Institut für Angewandte Analysis und Stochastik (WIAS), Berlin
  http://www.wias-berlin.de
  DFG Priority Program 1095
  "Analysis, Modeling and Simulation of Multiscale Problems"
  http://www.mathematik.uni-stuttgart.de/∼mehrskalen
  DFG Research Center MATHEON
  http://www.matheon.de

- **Organizers:**

  W. Dreyer (WIAS), B. Niethammer (Humboldt University of Berlin), J. Sprekels (WIAS)

- **Focus of the Workshop and Announced Topics**

  The workshop aims at bringing together researchers working on the following topics:

  - Discrete lattice models and their continuum limits
  - Discrete and continuum descriptions of nucleation and subsequent evolutions
  - Sharp interface limits of phase field systems

  Discrete lattice models serve as prototypes to study various possible limiting cases where a discrete ODE system can be substituted by a single or at least a few PDEs that describe the discrete dynamics on a continuum level.

  During the first stages of a phase transition small clusters of the new phase with Îś particles may grow or shrink by adding or subtracting a single particle. The evolution of the number of clusters is described by an ODE system of Becker-Döring type, which, however, should be substituted by a PDE if clusters above a certain size appear.

  Phase field systems resolve the interfacial region so that their evolution may be described by smooth fields. On the scale of microscopic observations the interfacial region mostly appears as a singular surface, where the observable fields change discontinuously. Thus the physical relevance of phase field systems is tested by their sharp interface limits.

- **Start:** May 29, noon
  End: June 01, noon
  Location: WIAS, Mohrenstr. 39, Berlin, Erhard-Schmidt-Hörsaal

Programme

Tuesday, May 29th

11:30 – 13:00	**Registration**
13:00 – 13:15	**Welcome**
13:15 –13:55	**A. Miranville**, Poitiers *Asymptotic behavior of Cahn-Hilliard-Gurtin equations*
14:00 – 14:40	**C. Kraus**, Berlin *Equilibrium conditions of liquid–vapour systems and the thermodynamical consistency of the van der Waals–Cahn–Hilliard phase model*
14:45 – 15:30	**Coffee Break**
15:30 – 16:10	**M. Röger**, Leipzig *The Allen-Cahn action functional and its sharp interface limit*
17:15 – 16:55	**B. Stinner**, Falmer *Systems of Allen-Cahn equations with volume constraints*
17:00 – 20:00	**Social Gathering**

Wednesday, May 30th

9:00 – 9:40	**C. Rohde**, Stuttgart *A numerical method for a sharp-interface model for phase transitions in compressible flow*
9:45 – 10:25	**L. Mugnai**, Leipzig *From atomistic to continuum models of elasticity and plasticity, "Kac-potentials" as an intermediate step*
10:30 – 11:00	**Coffee Break**
11:00 – 11:40	**A. Mielke**, Berlin *Weak convergence and homogenization in Hamiltonian systems*
11:45 – 12:25	**C. Patz**, Berlin *On dispersive stability of Hamiltonian systems on lattices*
12:30 – 14:00	**Lunch**
14:00 – 14:40	**P. Rosenau**, Tel-Aviv *Macro-complexity Micro-simplicity and vice versa: Problems and Paradoxes*
14:45 –15:25	**A. Vainstein**, Pittsburgh *Dynamics of steps along a martensitic phase boundary*
15:30 – 16:00	**Coffee Break**

Thursday, May 31st

9:00 – 9:40	**O. Kastner**, Bochum *Martensitic transformations in Lennard Jones Solids*
9:45 – 10:25	**T. Böhme**, Berlin *Determination of stiffness and higher gradient coefficients by means of the embedded atom method*
10:30 – 11:00	**Coffee Break**
11:00 – 11:40	**M. Hantke**, Magdeburg *On balance laws for mixture theories of disperse media with phase change*
11:45 – 12:25	**J. Velazquez**, Leipzig *Diffusive tails for the Becker-Döring model*
12:30 – 14:00	**Lunch**
14:00 – 14:40	**J. Wattis**, Nottingham *Self-similarity and scaling in nucleation problems*
14:45 –15:25	**M. Naldzhieva**, Berlin *Modeling and analysis of evolution of droplets*
15:30 – 16:00	**Coffee Break**
16:00 – 16:40	**C. Guhlke**, Berlin *Non-linear elastic membrane shells for incompressible Mooney-Rivlin materials and non-linear phenomena of rubber*
16:45 – 17:25	**B. Wagner**, Berlin *Sharp-interface models for dewetting films*

Friday, June 1st

9:00 – 10:30	**Time for Discussion**
10:30 – 11:10	**P. Rosenau**, Tel-Aviv *Macro-complexity Micro-simplicity and vice versa: Problems and Paradoxes. Part II*
11:15 – 12:30	**Time for Discussion**
12:30 – 12:15	**Closing**

Abstracts

Determination of stiffness and higher gradient coefficients by means of the embedded atom method

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For a quantitative theoretical description of phase separation and coarsening reliable data of stiffness constants and the so called Higher Gradient Coefficients (HGCs) are required. For that reason pair potentials of the Lennard-Jones type were used in [1] to provide a theoretical tool for their quantitative determination. Following up on this work these quantities are now calculated by means of the Embedded-Atom Method (EAM), a recently developed approach to describe interatomic potentials in metals. This is done, first, to achieve a better agreement between predicted and experimentally observed stiffness data as well as to avoid artifacts, such as the Cauchy paradox, and, second, to increase the trustworthiness of the HGCs for which experimental data are rarely available. After an introduction to the fundamentals of EAM it is outlined how it can be used for calculating stiffness constants and HGCs. In particular, Johnson's modification of EAM for nearest neighbor interactions [3] is applied to present explicit numerical results for a case study alloy, Ag-Cu, which has a "simple" face-centered-cubic crystal structure and where it is comparatively easy to obtain all the required analysis data from the literature and to experimentally compare the predictions of mechanical data.

Non-linear elastic membrane shells for incompressible Mooney-Rivlin materials and non-linear phenomena of rubber

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in preparation

On balance laws for mixture theories of disperse media with phase change

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To be announced

Martensitic transformations in Lennard Jones Solids

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Martensitic transformations (MT) are a special class of diffusion-less solid-solid phase transitions which occur in metallic alloys. This contribution shows results obtained from large scale atomistic simulations of MT in unconstrained test assemblies in 2D. The model employs binary Lennard-Jones potentials, which are constructed so as to allow for lattice transformations between a symmetric austenite phase and variants of martensite. With this model atom dynamic (AD) simulations concerning test assemblies of up to 262,000 atoms were carried out. The test assemblies had different rectangular shapes (bar-like to square). Constraints to the surface were minimized or absent (free surface) in order to allow for free nucleations and evolutions of MT. The simulations were carried out in temperature control mode in order to simulate temperature induced transformations. The results highlight the spatial and temporal evolution of MT in some detail. Observed phenomena are - the propagation of traveling transformation fronts across a bar, - the martensitic plate growth in extended bulk material involving the twinning process, - the free formation and accommodation of martensitic grain structures exhibiting different orientations.

Equilibrium conditions of liquid–vapour systems and the thermodynamical consistency of the van der Waals–Cahn–Hilliard phase model

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We first revisit the classical problem of liquid–vapour systems of a single substance at constant temperature. We assume that the two–phase system is contained in a vessel with a conserved total mass of the substance, whereby the vessel can be conducted at constant volume or at constant pressure. Our emphasis will be on the influence of different boundary conditions on the resulting equilibria for the van der Waals–Cahn–Hilliard model and the corresponding sharp interface model.
In the second part of the talk we show the compatibility of the van der Waals–Cahn–Hilliard phase model to the local version of the the second law of thermodynamics, i.e. to the local entropy inequality. It is well known, that the entropy inequality allows for the appearance of $\nabla\rho$ in the free energy only, if either the energy flux or the entropy flux is represented by a non-classical form. The various contributions to the balance of the internal energy are in principle directly measurable, whereas the entropy flux is not accessible to direct measurements. For this reason we prefer to preserve the classical form of the energy balance. We identify a non-classical entropy flux which admits higher-order gradient contributions in the free energy and in the Korteweg stress tensor.

Weak convergence and homogenization in Hamiltonian systems

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We present a general theory of weak convergence in the sense of Gamma limits for Lagrangian and Hamiltonian systems based on joint recovery operators. We derive conditions that guarantee that the limits of solutions of the parameter-dependent Hamiltonian systems solve the Hamiltonian system associated with the limiting Hamiltonian obtained independently via Gamma convergence.

We apply this theory to discrete, polyatomic oscillator chains and show that the limiting behavior is governed by a semilinear wave equation. The convergence in our rather weak setting allows for the treatment of general coefficients of L^∞ type, i.e. coefficients with jumps in the effective equations. This means that reflection and transmission at interfaces between different crystallographic phases is represented correctly by the weak solutions of the effective wave equation with nonsmooth coefficients.

Asymptotic behavior of Cahn-Hilliard-Gurtin equations

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To be announced

From atomistic to continuum models of elasticity and plasticity, "Kac-potentials" as an intermediate step

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Will be provided later

Modeling and analysis of evolution of droplets

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On dispersive stability of Hamiltonian systems on lattices

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We study the long-time dynamics of *oscillations in lattices of infinitely many particles* interacting via certain nonlinear potentials. In particular we consider the Klein-Gordon system on the infinite chain. The aim is to proof *dispersive stability* of such Hamiltonian systems analogously to results known for PDEs.

To do so we first recapitulate the dynamics of linear Hamiltonian systems on an infinite chain and give optimal decay rates based on the dispersion relation.

Based on this we proof that if the nonlinearity is weak enough, the Klein-Gordan system shows a similar behaviour like its linearisation.

A numerical method for a sharp-interface model for phase transitions in compressible flow

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The dynamics of a compressible fluid which occurs in a liquid and a vapour phase can be described on the continuum mechanical level as a free boundary problem where the bulk phases are governed by the Euler equations (or the Navier-Stokes equations in viscous media). As conditions at the free boundary mass conservation, the dynamic Young-Laplace law and an additional relation, sometimes called kinetic relation, are enforced. The kinetic relation can be seen as the up-scaled information from the microscopic level. From the numerical point of view the main difficulty is now the correct consideration of the pointwise conditions at the boundary. We present a ghostfluid algorithm combined with an almost classical Riemann-solver based finite volume technique that has the potential to handle such situations.

In the talk we will first discuss the analytical solution of the 1D-Riemann problem for the two-phase Euler equation which takes into account special kinetic relations at the phase boundary. Contrary to the classical gas dynamics for one-phase media the Riemann solution contains up to five single waves. The results rely on the work of Abeyaratne & Knowles and LeFloch et al. in the framework of elastodynamics. The Riemann solution is then a key stone to establish the ghostfluid/finite volume technique in the second part of the talk. We will present one- and twodimensional numerical simulations and a convergence proof for a simple but basic initial value problem. The third part of the talk will be devoted to a re-interpretation of the whole approach as a heterogeneous multi-scale method. In fact this different view allows to integrate the micro-scale information at the phase boundary in the numerical method not only in form of kinetic relations. It is quite naturally possible to integrate e.g. local computations with phase field models like the Navier-Stokes-Korteweg equations.

Macro-complexity Micro-simplicity and vice versa: Problems and Paradoxes

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will be provided later

The Allen-Cahn action functional and its sharp interface limit

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Stochastic perturbations of phase field equations allow for events that are out of the scope of deterministic models, as for example the switching between two stable states. Large deviation theory estimates the probability of such events in terms of a (deterministic) 'action functional'. Extending previous work by Kohn, Otto, Reznikoff and Vanden-Eijnden we consider the Allen-Cahn action functional in a particular scaling that exhibits a competition between nucleation and propagation costs. Our focus is on a lower bound that is sharp even in the case that higher multiplicities of the limiting phase interfaces occur. Our approach is based on techniques from Geometric Measure Theory and uses a generalized formulation of evolving hypersurfaces similar to that of Brakke for the mean curvature flow.

(joint work with Luca Mugnai)

Systems of Allen-Cahn equations with volume constraints

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Multi-phase systems are considered where the phase interfaces move according to a curvature flow and some of the phases are subject to volume constraints. An approximation of the free boundary problem by a phase field model has been developed resulting in parabolic differential equations with nonlocal terms due to the constraints. Several ideas will be presented to numerically solve the nonlocal equations, and simulations have been performed to study local minima of the system energy. Applications concern Wulff forms, bubble clusters, and tessellations problems.

Dynamics of steps along a martensitic phase boundary

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We study the motion of steps along a martensitic phase boundary in a cubic lattice undergoing antiplane shear deformation. We model a phase transforming material by assuming a stress-strain law that is piecewise linear with respect to one component of shear strain and linear with respect to another. Under these assumptions we derive a semi-analytical solution describing a steady sequential motion of the steps under an external loading. Our analysis yields kinetic relations between the driving force, the velocity of the steps and other characteristic parameters of the motion. We show that the kinetic relations are significantly affected by the material anisotropy. Our results indicate the existence of multiple solutions exhibiting sequential step motion.

Numerical simulations show that both subsonic and supersonic sequential propagation of steps can be stable. When the propagation speed exceeds a certain critical value that depends on anisotropy parameter, we observe a cascade nucleation of multiple steps which then join sequentially moving groups.

This talk is based on recent work with Yubao Zhen.

Diffusive tails for the Becker-Döring model

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Will be provided later

Sharp-interface models for dewetting films

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To be provided later

Self-similarity and scaling in nucleation problems

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