

Workshop “Phase Transitions and Optimal Control”
October 23 – 25, 2008

– *Abstracts* –

The periodic unfolding method as a mechanism to generate theorems

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We show how the periodic unfolding method can be used in conjunction with convergence or stability theorems in PDE’s to obtain new “homogenized” versions of these theorems. Several examples are given for linear and non linear elliptic PDE’s.

Error analysis for the elastic flow of parametrized curves

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We analyze a semidiscrete numerical scheme for approximating the evolution of parametric curves by elastic flow in \mathbb{R}^n . The fourth order equation is split into two coupled second order problems, which are approximated by linear finite elements. We prove error bounds for the resulting scheme and present numerical test calculations that confirm our analysis.

Optimal control of the propagation of a graph

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We study an optimal control problem for viscosity solutions of a Hamilton-Jacobi equation describing the propagation of a one dimensional graph with the control being the speed function. The existence of an optimal control is proved together with an approximate controllability result in the H^{-1} norm. We prove convergence of a discrete optimal control problem based on a monotone finite difference scheme and describe some numerical results.

Joint work with Klaus Deckelnick (Magdeburg) and Vanessa Styles (Sussex).

Modelling bioremediation of polluted soils

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Remediation of polluted soils can be carried out by means of bacteria able to metabolize specific pollutants attached to the soil grains. The bacteria can be floating in the water moving through the soil or they can attach to the solid skeleton forming a film. The presence of bacteria affects the rheological properties of the system. We examine the particular case of unsaturated soils, less treated in the literature.

Large deformations in mechanics

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Large deformations of solids are investigated. We use the polar decomposition of gradient matrix $\mathbf{F} = \mathbf{RW}$ (\mathbf{R} is rotation matrix, \mathbf{W} is stretch matrix). Large deformations of solids involve local spacial interactions either in an extension or in a rotation. Because local interactions are well described by spacial gradient: \mathbf{W} intervene for extensions and $\text{grad}\mathbf{R}$ intervene for rotations. Thus the free energy depends on \mathbf{W} and on $\text{grad}\mathbf{R}$. Moreover, free energy takes into account the volume impenetrability condition. Reactions to this impenetrability condition are important in constitutive laws. Within this point of view, self contact and extreme behaviors like the flattening (for example, solid flatten by a power hammer evolving from dimension 3 to dimension 2) are accounted for. With reasonable assumptions there exist non unique equilibrium positions.

On an energy model for nonlocal phase separation

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Equilibrium distributions in closed multicomponent systems maximize the entropy under the constraints of mass and energy conservation. In our talk we present an energy model for a multicomponent mixture of nonlocally interacting particles. Here, the nonlinear energy is given as the sum of the potential energy due to nonlocal interaction and the thermal energy of the ensemble. Based upon the iterative solution of the corresponding Euler-Lagrange equations, a direct ascent method for the entropy is established and applied to phase separation.

On a non-standard Allen-Cahn type problem

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We consider a two phase system where the physical variables (order parameter, chemical potential, and microentropy) satisfy suitable equations and relations. As the strong formulation of the problem is ill-posed, we consider a weaker version of it and transform the latter into an equivalent single equation for the order parameter, only. We essentially obtain an integrodifferential Allen-Cahn type equation and complement it with boundary and initial conditions. The present talk regards the results on well-posedness and long time behavior we have proved in a joint work in progress with P. Colli and J. Sprekels.

A potential theory for the boundary value problems of the unsteady equations of Stokes and Oseen

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The two most common linearizations of the Navier-Stokes' equations for incompressible fluid flow are those of Stokes and Oseen. In the late 1920s Lichtenstein and Odqvist simultaneously developed a potential theory for the steady systems of Stokes and Oseen. Motivated by the development of the theory of thermal potentials from that of the classical potential theory for the Laplace equation as well as more modern developments, we give here a potential theoretic approach to the boundary value problems for the unsteady systems of Stokes and Oseen.

On an inverse problem in fluid-structure interaction

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This lecture is based on a joint work with J. Elschner and A. Rathsfeld of WIAS in Berlin. It is concerned with an inverse scattering problem in fluid-structure interaction for construction the shape of the elastic scatterer from a knowledge of the far field patterns of the fluid pressure. We reformulate the problem as a nonlinear optimization problem including special regularization terms. We show that for any positive regularization parameter there exists a regularized solution minimizing the functional and that for the regularization parameter tending to zero, these regularized solutions converge to the solution of the inverse problem, provided the latter is uniquely determined by the given far field patterns. Some numerical experiments will be also included.

A variational inequality for grain boundary motion

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In this talk, a model for grain boundary motion, which was proposed by Kobayasi-Warren-Carter (KWC) in 2000 (*Physica D*, 140), is discussed from the mathematical point of view. In this model the two dimensional grain structure is described by two parameters, say, the mean orientation of crystalline and the degree of crystalline orientational order, as a polar coordinate system. Some interesting numerical experiences were given in the paper of KWC. But any theoretical treatment for this model has not been established because of some difficulties arising from the singular diffusivity and the degeneracy of mobility coefficient, etc. We shall try to overcome these difficulties by subdifferential approach.

Multigrid and phase field models

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The numerical solution of phase field models typically leads to large non-smooth algebraic systems which have to be solved approximately in each time step. We present multigrid methods for various Allen-Cahn and Cahn-Hilliard equations and discuss relations to optimal control and some practical applications.

Criteria for resonance in systems with Preisach nonlinearities

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We study forced periodic oscillations in systems with linear parts and Preisach nonlinearities. We suppose that equations of the systems depend on a scalar parameter and present almost necessary and sufficient conditions for existence of unbounded families of periodic oscillations. In particular, we compare our criterion with results following from well-known Changing Index Principle.

**Dynamical phase transitions and interface conditions
for two phase flows**

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Liquid vapor phase transitions can be modeled by the Navier-Stokes-Korteweg model, a modification of the compressible Navier-Stokes equations. In this case the equation of state is given by the van der Waals one. We will discuss the mathematical problems which arise from this system, some theoretical results and numerical simulations (together with Dennis Diehl). Furthermore we will discuss the behavior of static solutions of this model. One obtains that the pressure is continuous across the phase boundary although we expect that for the two phase flow the pressure is discontinuous across the interface between the phases and the jump is proportional to the mean curvature of the interface. But this is not a real contradiction since the pressure in the compressible and the incompressible Navier-Stokes equations are not the same. The classical relation between the mean curvature and pressure jump can be obtained by the low Mach number limit or for a suitable scaling of the capillarity coefficient in the Navier-Stokes-Korteweg model, at least for the static case. The last result we obtained together with C. Kraus and K. Hermsdörfer.

**Optimal control of parabolic variational inequalities
on bounded and unbounded domains**

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Optimal control of variational inequalities and the derivation of necessary optimality conditions remains to be a challenging topic. Our analysis is based, in part on Yosida type approximation to deal with both the case of bounded and unbounded domains. The unbounded domain case is motivated by problems in mathematical finance, for example. The main difficulty in this case results from lack of compactness in the Gelfand triple, so that the Aubin-Lions lemma is not applicable.

Numerical issues related to semi-smooth Newton methods and pathfollowing are also addressed.

Elastic free energies and statistical mechanics

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We show the relationship between lattice based Hamiltonians in equilibrium statistical mechanics and quasiconvex free energies in nonlinear elasticity.

Pseudoelasticity as limit of bistable chain with small viscosity

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Mechanical systems with so-called wiggly energies have many local equilibria. Under slow external forcing a gradient system with such an energy landscape may display rate-independent behavior. We discuss this phenomena that is claimed to be the origin of dry friction between bodies. In this talk we provide a mathematical justification of rate-independent one-dimensional pseudoelasticity as a limit for a chain of viscous, random, bistable springs, when the number of particles goes to infinity and the loading rate goes to 0.

(This is joint work with Lev Truskinovsky, Paris.)

The symmetric hyperbolic field equations in extended thermodynamics

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All field equations of thermodynamics are of balance type and – by the 2nd law – their solutions are supposed to satisfy the entropy inequality. This requirement entails that the field equations are symmetric hyperbolic. The symmetric hyperbolic structure ensures that the solutions have agreeable mathematical properties: well-posedness of initial value problems and finite characteristic speeds.

Fixed domain approaches in shape optimization problems

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Fixed domain methods have well-known advantages in the solution of variable domain problems including inverse interface problems. This paper examines two new control approaches to optimal design problems governed by general elliptic boundary value problems with Dirichlet boundary conditions. Numerical experiments are also included.

(Joint work with A. Pennanen and D. Tiba.)

Modelling of growth and transformations of complex structure in heterogeneous systems

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Dynamic developments of complex systems driven by multiply coupled mechanisms often contribute to formation of spatial patterns and non-uniform structures. This refers to various classes of biosystems, solid-state materials and, also structured interacting populations. Case study projects in mathematical modeling and computational simulation of such phenomena that have recently been studied at ICM will be reported.

Weak solutions to Frémond's full model of phase transitions

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The lecture is focused on the proof of existence of weak solutions for a 3D phase change model introduced by Michel Frémond in 2002. The result follows by passing to the limit in an approximate problem obtained adding a superlinear part (in terms of the gradient of the temperature) in the heat flux law. We show that at the limit the total energy is conserved during the evolution process and prove the non-negativity of the entropy production rate in a suitable sense. Finally, these weak solutions turn out to be the classical solution to the original Frémond's model provided all quantities in question are smooth enough.

The results are contained in a recent joint work with Eduard Feireisl and Hana Petzeltová, which is the preprint no. 2008-009 of the Nečas Center for Mathematical Modeling and it is going to appear in Math. Methods Appl. Sci.

On an evolution quasi-variational inequality with gradient constraint

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We prove the existence of variational solutions for an evolution quasi-variational inequality in a class of convex sets characterized by a constraint on the absolute value of the gradient that depends on the solution itself. The only required assumption on the nonlinearity of this constraint is its continuity and positivity. The method relies on an appropriate parabolic regularization and suitable "a priori" estimates. This is a joint work with Lisa Santos.

Shape optimization for compressible Navier-Stokes equations

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For drag minimization problem the theoretical results are presented including the existence of optimal shapes of an obstacle, the necessary optimality conditions, and the framework for the level type method for numerical solution. The theoretical results are obtained in the framework of collaboration with P.I. Plotnikov (Novosibirsk). The numerical part is developed in collaboration with A. Zochowski (Warsaw).

Reference

- [1] P.I. Plotnikov, J. Sokołowski, Stationary Boundary Value Problems for Compressible Navier-Stokes Equations, in: Handbook of Differential Equations, Vol. 6, M. Chipot (Ed.), Elsevier, 2008.

Optimization of thin elastic structures

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We present results concerning the optimization of the thickness or of the shape for thin elastic structures like beams, plates, arches, curved rods, shells. We discuss subjects related to existence, optimality conditions, approximation, numerical experiments and examples. They have been investigated in a sequence of papers due to J. Sprekels, D. Tiba, and their collaborators. As a strongly related subject, we shall also present the application of the control variational method to Kirchhoff-Love arches and to simplified models of plates. Much of the material may be found in the recent monograph of P. Neittaanmäki, J. Sprekels, D. Tiba “Optimization of elliptic systems. Theory and applications”, Springer, New York (2006).

**Convergence to equilibrium for parabolic-hyperbolic time-dependent
Ginzburg-Landau-Maxwell equations**

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This is a recent joint work by M. Grasselli, H. Wu, and S. Zheng. In this paper we consider a Ginzburg-Landau-Maxwell model which describes the behavior of a two-dimensional superconducting material. Under the choice of Coulomb (i.e., London) gauge, the resulting system is a parabolic-hyperbolic coupled system of nonlinear partial differential equations subject to suitable boundary and initial conditions. Global well-posedness results were proved by M. Tsutsumi and H. Kasai (1999), while the existence of global attractor and exponential attractors was proved by V. Berti and S. Gatti (2006). In this paper we use an extended Łojasiewicz-Simon approach to show that for any initial datum in certain phase space, the corresponding global solution converges to an equilibrium as time goes to infinity. Besides, we also provide an estimate on the convergence rate with respect to the phase space metric.