BMS Summer School 2014[1]

Applied Analysis for Materials

25 August – 5 September

Abstracts of Minicourses

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Uwe Bandelow (WIAS)

Basic equations of classical soliton theory: solutions and applications

Nonlinear waves appear in many disciplines of science and represent an important frontier for the understanding of Nature. Tidal waves and Tsunamis are known since hundreds of years. After a gestation period of about 150 years the soliton concept has been established, which describes long-living nonlinear waves with invariable shape and robustness in scattering. Different kinds of solitons have been observed experimentally in various real systems, as in hydrodynamics, particle physics, and optics.

The lecture will introduce three different basic equations that allow for soliton solutions, namely,

1. Korteweg-de Vries-Equation (KdV), originally derived for flat water waves:

$$\frac{\partial u}{\partial t} + 6u\frac{\partial u}{\partial x} + \frac{\partial^3 u}{\partial x^3} = 0,$$

2. Sinus-Gordon-Equation, originally derived for lattice waves:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + \sin u = 0,$$

3. Nonlinear Schrödinger-Equation, suited for wave enveloppes:

$$i\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial x^2} + |u|^2 u = 0.$$

Exact analytic soliton solutions for these equations will be calculated during the lecture. Furthermore, transformation methods will be provided, which allow for the calculation of exact higher-order soliton solutions that allow to study scattering processes. In the last lecture, the inverse scattering theory will be introduced, which is a general method for the calculation of exact solutions of such completely integrable equations, and applied at hand of the KdV.

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Dietmar Hömberg (WIAS)

Optimal control and shape design problems in thermomechanics

Many technological processes can be described by partial differential equations. For many years the role of industrial and applied mathematics was mainly to try to understand the respective process, to derive and analyse an appropriate PDE or ODE model for it and to simulate it using, e.g., a finite-element approximation. However, the ultimate goal usually is to try to optimise the process. Mathematically, this requires the solution of an optimal control problem, i.e., a constrained nonlinear optimization problem in which the constraints are PDEs. In the first part of my lectures I will review the basic theory of pde-constrained control. We will derive optimality conditions of first and second order and discuss numerical solution strategies. While the control in the first part typically is either a coefficient or an inhomogeneity of the considered PDE, in optimal shape design problems, the shape of the domain or of an interface acts as the control. In the second part of my lectures we will investigate a mechanical shape design problem related to a solid-solid phase transition. We will discuss optimality conditions and derive a numerical solution strategy based on a phase field regularisation.

Dorothee Knees (Universität Kassel)

Evolutionary variational inequalities in the context of inelastic solids

Everyone might already have done the following experiment: when pulling a slide via a spring over a rough surface, first the spring stretches before the slide starts to glide. Knowing the time-dependent position of the tip of the spring one is interested in an evolution model that describes the forces in the spring and the motion of the slide. Since the slide does not move until the forces acting on it reach a certain threshold, we are led to evolutionary variational inequalities.

The lecture series is devoted to the analysis of evolutionary variational inequalities arising in the modeling of inelastic solids. In the framework of standard generalized materials it is assumed that the state of a body is completely characterized by the displacements u (the position of the tip of the spring in the previous example) and internal variables z (the position of the slide; more general: plastic strains, damage or crack variables, phase variables in the context of shape memory alloys). Further it is assumed that the evolution law can be deduced from a time dependent stored energy functional $\mathcal{E}(t,u,z)$ (e.g., accounting for the elastic energy stored in the spring) and a dissipation potential $\mathcal{R}(\dot{z})$ in the sense that during the evolution the thermodynamical driving forces $-\mathrm{D}_z\mathcal{E}(t,u(t),z(t))$ and the internal friction forces $\partial\mathcal{R}(\dot{z})$ are in equilibrium. This leads to the equations

$$\begin{aligned} 0 &= \mathrm{D}_u\mathcal{E}(t,u(t),z(t)) \\ 0 &\in \partial\mathcal{R}(\dot{z}(t)) + \mathrm{D}_z\mathcal{E}(t,u(t),z(t)). \end{aligned}$$

Due to constraints (like the threshold in the slide example) the second relation in general is an evolutionary variational inequality and $\partial\mathcal{R}(\dot{z})$ denotes the subdifferential of $\mathcal{R}$.

The lecture courses focus on the following topics:

- Modeling of inelastic material behavior
- Equivalent formulations of the evolution law
- Existence of solutions (in function spaces)
- Discussion of specific examples and extensions

Claude Le Bris (CERMICS - ENPC)

Nonperiodic homogenization of elliptic equations: stochastic and deterministic approaches

We review some recent developments in theoretical and computational nonperiodic homogenization. The results have been obtained in a series of works with X. Blanc (Paris 7), PL Lions (College de France), F. Legoll (Ecole des Ponts and Inria) and various other collaborators. The methods devleoped all aim at designing numerical approaches that both are practically relevant and keep the computational workload limited.

Alexander Mielke (WIAS)

Multiscale modeling and evolutionary Gamma-convergence for gradient flows

A gradient system is a triple consisting of a state space, an energy functional $\mathcal{E}$ and a dissipation potential Ψ. The gradient flow is generated by the evolution equation defined via

$$0 = \mathrm{D}\Psi(\dot{u}(t)) + \mathrm{D}\mathcal{E}(u(t))$$

We consider the case of parameter dependent gradient systems $(X, \mathcal{E}_\varepsilon, \Psi_\varepsilon)$ and discuss the question whether the convergence of the two functionals to limit functionals induces the convergence of the solutions of the evolution equations.

We discuss the notions of Γ, Mosco and continuous convergence and provide different techniques to derive corresponding convergence results for the solutions. This includes De Giorgi's *energy-dissipation formulation* for gradient flows as well as the *integrated evolutionary variational estimate* for abstract metric gradient systems. We also discuss the relevance of well-preparedness of initial conditions.

Christoph Ortner (Warwick University)

Atomistic/Continuum Multiscale Methods

A/c methods are a class of computational multiscale schemes that combine the accuracy of atomistic models with the efficiency of continuum elasticity. They are increasingly utilized in materials science to study the fundamental mechanisms of material failure such as crack propagation and plasticity, which are governed by an interaction between crystal defects and long-range elastic fields.

The in the construction of a/c methods various approximation errors are committed. In these lectures I will introduce a rigorous numerical analysis approach that classifies and quantifies these errors and which can therefore give confidence in the simulation results, as well as enable optimisation of the numerical methods for accuracy and computational cost.

Topics I plan to cover: Cauchy-Born continuum model, atomistic description of defects in a homogeneous host crystal, a/c coupling via blending, consistency and stability, outlook towards schemes incorporating finite-temperature and/or electronic structure.

Mark A. Peletier (TU Eindhoven)

Stochastic origins of energies and gradient flows: a modelling guide

In equilibrium systems there is a long tradition of modelling systems by postulating an energy and identifying stable states with local or global minimizers of this energy. In recent years, with the discovery of Wasserstein and related gradient flows, there is the potential to do the same for time-evolving systems with overdamped (non-inertial, viscosity-dominated) dynamics. Such a modelling route, however, requires an understanding of which energies (or entropies) drive a given system, which dissipation mechanisms are present, and how these two interact. Especially for the Wasserstein-based dissipations this was unclear until rather recently. In this series of talks I will build an understanding of the modelling arguments that underlie the use of energies, entropies, and gradient flows. This understanding springs from the common connection between large deviations for stochastic particle processes on one hand, and energies, entropies, and gradient flows on the other. I will explain all these concepts in detail in the lectures.