University Center for Mathematical Modeling, Applied Analysis and Computational Mathematics

Semester Seminar, 26$^{\text{th}}$ June 2017, 8:30–12:30, Room K6

Schedule

Time	Speaker	Title
8:30		Opening
8:30	Benjamin Vejnar	A Sobolev homeomorphism in four dimensions
8:50	Dušan Pokorný	Integral geometry of WDC sets
9:10	Marek Cúth	Finitely additive measures and complementability of Lipschitz-free spaces
9:30		Coffee Break
9:40	Michal Pavelka	Implicit constitutive relations by means of gradient dynamics
10:00	Klára Kalousová	Transfer of heat and liquids through the high-pressure ice layer of Ganymede
10:20	Ondřej Souček	Heterogeneous catalysis
10:40	Karel Tůma	New understanding of a classical Burgers model and its usage in a simulation of a wheel tracker test of asphalt concrete
11:00		Coffee Break
11:10	Miloslav Vlasák	A posteriori error estimates for evolution problems with conforming discretizations
11:30	Martin Lanzendörfer	Introducing a coupled PDE/ODE approach into pharmacokinetic/pharmacodynamic modelling for dosage regimen
11:50	Václav Vlasák	The sizes of the classes of $H^{(N)}$ sets
12:10		Conclusion

Abstracts

Benjamin Vejnar: A Sobolev homeomorphism in four dimensions. For $n \geq 4$, we sketch a construction of a homeomorphism f in the Sobolev space $W^{1,1}((0,1)^n, \mathbb{R}^n)$ whose Jacobian is positive on a set of positive measure and also negative on a set of positive measure. This solves a problem of Hajlasz. It is known that such a homeomorphism can not exist in dimension $n \leq 3$. It follows by the properties of f that it can not be approximated by diffeomorphisms (or by piecewise affine homeomorphisms) in $W^{1,1}_{\text{loc}}$. This is a joint work with S. Hencl.

Dušan Pokorný: Integral geometry of WDC sets. During the last five years the curvature theory for a newly defined class of the so-called WDC sets has been developed. Those results generalize in a substantial way the previous theory (namely the case of the sets of positive reach) and include the proof of the existence of the of curvature measures for the WDC sets (Pokorný, Rataj 2013) and the validity of the kinematic formulas (Fu, Pokorný, Rataj 2017), results already presented at previous MathMAC seminars, as well as some recent results on the structure of WDC sets by Pokorný, Rataj, Zajíček (preprint 2017) and the extension of the theory for the class of U_{WDC} sets, which finally subsumes also the important case of the convex ring.

In the talk, I will try to explain the main purposes of the (modern) curvature theory and the role of our results in the whole framework.

Marek Cúth: Finitely additive measures and complementability of Lipschitz-free spaces. Given a metric space M it is possible to construct a Banach space $F(M)$ in such a way that the metric structure of M corresponds to the linear structure of $F(M)$. This space $F(M)$ is sometimes called the Lipschitz-free space over M. The study of Lipschitz-free spaces is well-motivated: for example, if we knew that $F(\ell_1)$ is complemented in its bidual, it would solve famous open problem of whether every Banach space which is Lipschitz-isomorphic to ℓ_1 is actually linearly isomorphic to ℓ_1.

I will talk about our recent paper with O. Kalenda and P. Kaplický, where we prove that $F(\mathbb{R}^n)$ is complemented in its bidual.

Michal Pavelka: Implicit constitutive relations by means of gradient dynamics. Gradient dynamics, where thermodynamic fluxes are given as derivatives of a dissipation potential with respect to thermodynamic forces, is a geometrical way for obtaining constitutive relations. The geometrical structure enables us to formulate the conjugate gradient dynamics by means of Legendre transformation. The conjugate gradient dynamics then gives forces as functions of fluxes, which can be interpreted as implicit constitutive relations. Moreover, the conjugate representation makes it possible to lift the dynamics to an extended level of description, where stability, metastability and instability of the dynamics can be revealed by straightforward thermodynamic arguments.

Klára Kalousová: Transfer of heat and liquids through the high-pressure ice layer of Ganymede. The exploration of ocean worlds—planets or moons that harbor subsurface oceans—is prompted by the question of the emergence of life in places where liquid water is present. A lot of attention is given to Europa and Enceladus where the deep ocean is expected to be in a direct contact with the silicate mantle—such conditions are similar to those at terrestrial sea floors where life develops. Ganymede, the largest moon in the solar system, possesses a larger amount of H2O so that a layer of high-pressure (HP) ice exists in its interior that seems to prevent the direct contact of water with silicates. We study the dynamics of Ganymede's HP ice layer by solving the conservation equations of mass, momentum, and energy of a two-phase mixture by the finite element method. Our results suggest that melting can occur at the silicate/HP ice interface and that the melt is then transported through the layer by the upwelling plumes. Depending on the vigor of convection, it stays liquid or it may freeze before melting again as the plume reaches the partially molten layer at the top boundary from where it is extracted into the ocean.

Ondřej Souček: Heterogeneous catalysis. We present a phenomenological derivation of a thermodynamically consistent continuum-mechanics model of heterogeneous catalysis for a multicomponent fluid solution with adsorption onto a solid surface. The model involves mass and heat transport phenomena for chemically reacting multicomponent bulk and surface phases including mutual mass exchange between the phases, so-called sorption. The derivation stems from a specification of thermodynamic potentials (free energies) of the mixture in the bulk (in an ideal mixture form) and on the active surface (deduced from a certain simplified lattice structure model) and from the specification of the entropy production both in the bulk and on the active surface.

Karel Tůma: New understanding of a classical Burgers model and its usage in a simulation of a wheel tracker test of asphalt concrete. A classical Burgers model can be understood as an incompressible rate-type fluid model for viscoelastic material in which every material point reacts as it consisted of two Maxwell-like elements. They behave such that the elastic part of response (compressible neo-Hookean) together with the dissipative part creates an incompressible connection. The full three-dimensional model is derived using the thermodynamical approach that employs the notion of natural configuration to split the total deformation into the purely elastic part and the dissipative one. In case of the Burgers model the two natural configurations are used to fit a complicated response caused by at least two different relaxation mechanisms observed in the asphalt.

The group of J. Murali Krishnan from Indian Institute of Technology studied the response of the asphalt concrete in a wheel tracker test, a long torture experiment to study the abilities of a newly designed material. The new understanding of the Burgers model says how to formulate this second order model using two symmetric first order governing equations, and with this we simulated the wheel tracker test.

Miloslav Vlasák: A posteriori error estimates for evolution problems with conforming discretizations. We will consider a simple heat equation as a well understood representative of parabolic PDEs. We will assume conforming finite element discretization in space coupled with either conforming or nonconforming higher order Galerkin time discretizations. For the resulting scheme we will present guaranteed, cheap and fully computable a posteriori error upper bound. Moreover, we will show that this upper bound is locally efficient. This concept can be applied to some specific simplified situations, e.g. ODEs, as well as generalized to nonconforming space discretizations or nonlinear PDEs.

Martin Lanzendörfer: Introducing a coupled PDE/ODE approach into pharmacokinetic/pharmacodynamic modelling for dosage regimen. The standard mathematical modelling technique used in state-of-the-art dosage regimen research in pharmacology is based on the concept of several interconnected compartments (such as blood, tissue, cytoplasm, nucleus), the concentrations of all tracked metabolites being considered roughly constant in each compartment, so that one can describe the evolution of all concentrations by a system of ODEs in time. We will discuss a new approach, emerging in this context only recently, in which the space-resolution within some of the compartments is included, the resulting model being a coupled system of several ODEs and reaction-diffusion PDEs. This is a work in early progress; we will discuss the need for such an approach and the challenges to be expected: both mathematical and interdisciplinary. Joint work with M. Azar, J. Duintjer Tebbens, P. Pavek (FaF UK).

Václav Vlasák: The sizes of the classes of $H^{(N)}$ sets. I will speak about sets of uniqueness for trigonometric series and some of its interesting subcollections mainly $H^{(N)}$ sets. I will discuss several problems related to polars of those collections. I will present the result that polars of collections of $H^{(N)}$ sets are different for every N.