University Center for Mathematical Modeling, Applied Analysis and Computational Mathematics

Semester Seminar, hybrid form (in person and via Zoom),
Room K3, Wednesdays, November 22 and 29 and December 13, 09:00-10:20

Schedule

Time	Speaker	Title
Nov 8		
9:00–10:30	Nadine Cetin	Introduction to Quantum Fluids
Nov 22		Chair: Karel Tůma
9:00–9:05		Opening
9:05–9:25	Petr Pelech	Stress-mediated growth determines E. Coli division site morphology
9:25–9:45	Vojtěch Patočka	Dynamic component of the asthenosphere: dislocation creep at the base of subducting slabs
9:45–10:05	Stefano Pozza	A new fast numerical method for the generalized Rosen-Zener model
10:05–10:20		Closing
Nov 29		Chair: Josef Málek
9:00–9:05		Opening
9:05–9:25	Petr Šácha	Numerical experiments produced by the Gravity wave research group at KFA MFF UK
9:25–9:45	Jan Blechta	Quasi-optimal Discontinuous Galerkin discretisations of the p-Dirichlet problem
9:45–10:05	Lenka Slavíková	Strongly nonlinear Robin problems for harmonic functions in the half-space
10:05–10:20		Closing
Dec 13		Chair: Josef Málek
9:00–9:05		Opening
9:05–9:35	Ondřej Chrenko	Observational signatures of vortex-driven planet migration
9:35–10:05	Michal Pavelka	Recognition of Hamiltonian models by machine learning
10:05–10:20		Closing
Dec 20		
9:00–10:30	Jiří Zeman	Machine Learning Effective Models of Interfacial Interactions

Abstracts

Jan Blechta: Quasi-optimal Discontinuous Galerkin discretisations of the p-Dirichlet problem. The classical arguments employed when obtaining error estimates of Finite Element (FE) discretisations of elliptic problems lead to more restrictive assumptions on the regularity of the exact solution when applied to non-conforming methods. The so-called minimal regularity estimates available in the literature relax some of these assumptions, but are not truly of minimal regularity, since a data oscillation term appears in the error estimate. Employing an approach based on a smoothing operator, we derive for the first time error estimates for Discontinuous Galerkin (DG) type discretisations of non-linear problems with (p, δ)-structure that only assume the natural $W^{1,p}$-regularity of the exact solution, and which do not contain any oscillation terms.

This is a joint work with Alexei Gazca, Alex Kaltenbach, and Michael Růžička.

Nadine Cetin: Introduction to quantum fluids. Helium is the only known element which remains liquid when it is cooled down. At a certain temperature T Helium undergoes a phase transition and becomes a so—called quantum liquid. In this state it is a treasure box for physicists as it requires bringing together many fields of theoretical physics for its understanding. There exist up to date many models for describing its various fascinating properties like superfluidity or the presence of quantized vortices. The latter are singularities in the fluid at which the rotation of the superfluid velocity v_s does not vanish, although it should be a potential flow according to the models. In this talk the physical properties of superfluid helium will be presented, and the two–fluid model will be introduced, on which all further models are more or less based. Since superfluid Helium is a quantum system, it should be understood on the basis of quantum mechanical principles. This has first been done by L. Landau in 1947 who gave with that a microscopic foundation of the hydrodynamic (macroscopic) equations of superfluid Helium. However, up to now it has not been possible to include the dynamics of quantized vortices from scratch, and hence a complete and fundamental understanding based quantum mechanics seems to be still lacking. After a short recap of the basics of quantum mechanics I will present the questions I will be working on in the upcoming months. These include amongst others: how are the different models related? Is it possible to introduce the dynamics of quantized vortices into the models on the basis of quantum mechanical principles? Is many—body quantum mechanics enough or is a description by full quantum field theory necessary?

Ondřej Chrenko: Observational signatures of vortex-driven planet migration. A giant planet embedded in its natal protoplanetary disk can open a gap along its orbit. It has been recently proposed (Lega et al. 2021) that if the gas disk is inviscid, a large-scale vortex can form at the outer edge of the planet-induced gap and regulate the planet's radial migration. Later on, the vortex flattens the outer gap edge and eventually decays, leaving the gap asymmetric. Motivated by the fact that both the gap edge and the vortex have an ability to accumulate drifting dust grains, we perform 3D multifluid gas-dust simulations of vortex-driven planet migration with the aim to predict observational signatures of this process from the thermal emission of dust grains that can be detected e.g. by the radio interferometer ALMA. In my seminar contribution, I will outline the first results of this project.

Vojtěch Patočka: Dynamic component of the asthenosphere: dislocation creep at the base of subducting slabs. Defined as a mechanically weak layer that accommodates vertical isostatic movements of continents, asthenosphere is an old geodynamic concept (Barrell, 1914). The asthenosphere plays a crucial role in the theory of plate-tectonics as it is responsible for transferring stresses to/from tectonic plates (Forsyth et al., 1975), but its origin remains uncertain. Two prevailing theories are that it is a region where plumes hotter than an average mantle spread below the lithosphere, forming a global layer of elevated temperature and thus small viscosities (e.g., Morgan et al., 2013), or that it is the change in the water content that softens the sublithospheric mantle (e.g., Karato, 2012). The common assumption is thus that the asthenosphere is of thermal and/or compositional origin. Here we explore sublithospheric weakening due to dislocation creep at the base of subducting plates, activated by the high strain-rates that result from the motion of tectonic plates relative to the mantle (dynamically generated asthenosphere).

Early studies on rock deformation indicated that dislocation creep dominates over diffusion creep throughout the upper mantle. The idea of dislocation creep in the asthenosphere thus comes from re-evaluating the importance of diffusion creep in the shallow and the deeper mantle, and is relatively old (Karato and Wu, 1993). Nevertheless, the ratio of dislocation to other creep mechanisms has not been systematically evaluated in models of plate-like mantle convection. We use numerical simulations of subduction to estimate the contribution of dislocation creep to sublithospheric weakening. Depending on parameters of the subducting slab, namely the velocity, age, and the stage of subduction, the mantle below oceanic plates and in the mantle wedge may be significantly dynamically weakened, with dislocation creep viscosity being smaller than that of diffusion creep by more than an order in magnitude. We do not argue against thermal or compositional effects – the different weakening mechanisms are likely superimposed.

Michal Pavelka: Recognition of Hamiltonian models by machine learning. Imagine you have some data as a sequence of snapshots (state vectors) of a mechanical system in time. How to find out what kind of mechanical system has generated the data? In order to answer that question, we need the differential equations that describe motion of that system. Machine learning (Direct Poisson Neural Networks) provides means to recover the Hamiltonian form of that equations (the underlying Poisson bracket and Hamiltonian) from the snapshots. This technique also distinguishes between symplectic and non-symplectic mechanical systems and, moreover, it can tell whether the system is Hamiltonian at all. This is a joint work with Martin Šípka, Ogul Esen, and Miroslav Grmela.

Petr Pelech: Stress-mediated growth determines E. Coli division site morphology. Unlike human cells, the bacterial cell wall is strengthened by a peptidoglycan (PG) matrix, a large polysacharide, which acts as an exoskeleton, provides protection from external stressors, and protects the bacteria from osmotic lysis; the PG wall synthesis is therefore a natural target of penicillin based antibiotics. As the PG macromolecule is rather rigid when compared to forces exerted by proteins, the mechanical explanation of the wall's remodeling process during the bacterial division is a challenging task. And although the protein complexes responsible for the wall's remodeling have been identified and described in detail, the exact role of particular components, their precise cooperation, and the interaction with the inner and outer cell membrane still remain poorly understood.

Our collaboration possesses unique data resulting from a combination of genetic engineering and cryoelectron tomography [1]. Cells with modified genomes evince different division dynamics that lead to untypical shapes and bacterial morphology. To supplement the static images with an insight into a hypothetical evolution, we have developed a continuum model of stress mediated bacterial growth within the framework of morphoelasticity [2].

By comparison with measurements of cell lysis we have found a plausible range of (internal) turgor pressure and elastic moduli of the PG matrix, whose values reported in the literature vary by several orders of magnitude. By modifying the remaining growth parameter we have succeeded in reproducing an altered cell's morphology at the division site, which resembles the shape of mutated bacteria.

[1] Navarro, P.P., Vettiger, A., Ananda, V.Y. et al. Cell wall synthesis and remodelling dynamics determine division site architecture and cell shape in Escherichia coli. Nat Microbiol 7, 1621–1634 (2022). https://doi.org/10.1038/s41564-022-01210-z

[2] Goriely, Alain, and Derek Moulton, '6 Morphoelasticity: A theory of elastic growth', in Martine Ben Amar and others (eds), New Trends in the Physics and Mechanics of Biological Systems: Lecture Notes of the Les Houches Summer School: Volume 92, July 2009, Lecture Notes of the Les Houches Summer School (Oxford, 2011; online edn, Oxford Academic, 22 Sept. 2011), https://doi.org/10.1093/acprof:oso/9780199605835.003.0006

[3] Ganhui Lan, Charles W. Wolgemuth, and Sean X. Sun. (2007). Z-ring force and cell shape during division in rod-like bacteria. PNAS 104 (41) 16110-16115. https://doi.org/10.1073/pnas.0702925104

[4] Nguyen, L.T., Oikonomou, C.M., Ding, H.J. et al. Simulations suggest a constrictive force is required for Gram-negative bacterial cell division. Nat Commun 10, 1259 (2019).

Stefano Pozza: A new fast numerical method for the generalized Rosen-Zener model. In quantum mechanics, the Rosen-Zener model represents a two-level quantum system. Its generalization to multiple degenerate sets of states leads to larger non-autonomous linear system of ordinary differential equations (ODEs). We propose a new method for computing the solution operator of this system of ODEs. This new method is based on a recently introduced expression of the solution in terms of an infinite matrix equation, which can be efficiently approximated by combining truncation, fixed point iterations, and low-rank approximation. This expression is possible thanks to the so-called $*$-product approach for linear ODEs. In the numerical experiments, the new method's computing time scales linearly with the model's size. We provide a first partial explanation of this linear behavior. Joint work with Christian Bonhomme and Niel Van Buggenhout.

Lenka Slavíková: Strongly nonlinear Robin problems for harmonic functions in the half-space. In this talk, we will discuss the existence and global regularity of harmonic functions, in n-dimensional half-spaces, subject to general nonlinear Robin type boundary conditions. Our main focus will be on nonlinearities of exponential type, which arise naturally in connection with problems in conformal geometry and electrochemistry; our approach will however be general enough to cover a wide range of different nonlinearities. Function spaces defined in terms of Orlicz norms will play an essential role in our discussion. This is a joint work with Andrea Cianchi and Gael Diebou Yomgne.

Petr Šácha: Numerical experiments produced by the Gravity wave research group at KFA MFF UK. In this talk we will introduce the modeling tools that we use in our research group, including detailed description of the set of governing equations and their discretization, and demonstrate their utility for the scientific questions that we tackle.

Jiří Zeman: Machine Learning Effective Models of Interfacial Interactions. Abstrakt: Cell membranes tend to interact with electrolyte that surrounds them and electrostatic effects due to the presence of ions are crucial to maintain important functions in living organisms, such as communication between tissues or signal propagation in the human brain. Certain ions have a stabilizing effect on macromolecules and are therefore called cosmotropic (order-creating), whereas others, called chaotropic, disrupt hydrogen bonds, which may lead to protein denaturation. Proper description of these properties is valuable from the application perspective even for more simple systems, such as an oil-water interface that we have studied recently. First, an overview of the topic will be given in this talk to make the subject accessible to a possibly wider audience. Second, the sketch of an ML-inspired modelling approach to ion adsorption will be discussed. Based on preliminary investigations with Christoph Allolio.