

Postdoc position at Czech Technical University in Prague, Faculty of Nuclear Sciences and Physical Engineering, Department of Mathematics

Mathematical Modelling and Numerical Simulation of Phase Transitions in Crystalline and Porous Materials

Brief description

Maximal duration: until December 31 2022

Beginning: upon personal preference

Funding: Ministry of Education of Czech Republic

Suitable for postdoc or early-career researchers

Contents: joint research work on mathematical and numerical modelling of phase transitions with the Mathematical Modelling Group of the Department of Mathematics

<http://geraldine.fjfi.cvut.cz>

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This information is posted on: http://geraldine.fjfi.cvut.cz/mmg/files/postdoc_19.pdf

Details

Investigation of free-boundary problems has been developed during last decades as a consequence of problems solved in physical or biological contexts, achieved advances in material science, space technology and fluid dynamics. Free boundaries are frequently understood as hypersurfaces described by geometrical means, which dynamically evolve due to the driving forces arising in governing partial differential equations. The entire problem becomes nonlinear and its mathematical treatment non-trivial. Closer analysis of these problems and their role in mathematical modelling lead to further improvements including incorporation of anisotropy as additional feature of the environment (crystalline lattice or surfacial energy density). Description of anisotropy, namely in three-dimensional space, reflecting real symmetries and allowing mathematical analysis of the problem simultaneously represents a separate branch of research.

In the project, a class of moving boundary problems will be investigated. It is assumed that such problems are described by the law for the normal velocity of the interface incorporating mean curvature, Gaussian curvature and their differentials. The research in progress is carried out for the problems of pure advection used for fluid-component tracking, for the problems of curvature-dependent evolution up to the problems of surface diffusion. The scope of the law within the project will encompass the following particular cases: mean-curvature flow relating the normal velocity of the interface to its mean curvature, constrained mean-curvature flow preserving the area enclosed by the interface, surface diffusion containing the surface Laplacian of curvature.

The mathematical treatment of the motion law relies either on methods directly tracking the position of or on methods which yield the position of the interface as a consequence of the solution of a higher-dimensional problem. In any case, it leads to analysis of nonlinear degenerate partial differential equations, mostly of parabolic type.

Connection of the above described class of moving-boundary problems can be found in many areas of science. The below listed examples are related to the scope of the project. Variety of free-interface phenomena accompany processes in the material science. The solidification process in case of a pure substance is described by the modified Stefan problem. The mentioned problem contains the motion

law at the phase boundary in the form of the Gibbs-Thomson relation. Redistribution of the grain boundaries in a solid material is governed by a dependence on the second derivative of curvature along the interface. Elastic effects in materials such as thin-layer development and fracture are described by the surface-diffusion law. Curves of crystalline dislocations also move with a dependence on curvature within the dislocation planes. The topic finds a rich application in computer image processing. e.g. in medical context.

The mentioned problems involve the motion law for the hypersurface or curve together with a conservation law for energy, mass of particular components etc. In this sense, complete analysis of any such problems still remains a challenge. Another area of wide application for moving-fronts algorithms is the simulation of porous-media flow of multiple phases and their transitions. A careful experimental investigation has discovered fingering phenomena accompanying the transport of non-aqueous phase liquids (NAPLs) in the interaction with the wetting phase (usually water). Complicated patterns of the NAPL phase develop during the interaction with pores and other phases, and are a result of the nonlinear behavior of governing equations. The phenomenon can be described by the Hele-Shaw problem for the pressure and position of the phase interface. In case of low influence of capillarity effects, the multi-phase flow is described by a nonlinear conservation law known as Buckley-Leverett problem. Recently, the research interest started to focus on the soil freezing and thawing within the context of climatic changes worldwide where especially the permafrost thaw leading to the release of large amount of gases becomes worth of investigation.

The research team in the Department of Mathematics, Faculty of Nuclear Sciences and Physical Engineering, CTU in Prague has long term contacts and personal exchange including former postdoc stays at the CTU with research institutions abroad dealing with moving boundary problems in continuum mechanics and similar problems such as Meiji University, Tokyo, Kanazawa University and University of Miyazaki, Japan within the context of anisotropic free-boundary problems, UCLA Los Angeles within the context of surface diffusion, Colorado School of Mines, Golden – flow, transport and phase transitions in porous media, and the Paris Sud Orsay for planar curve dynamics and applications.