ParaPhase: Towards HPC for adaptive Phase-Field Modeling

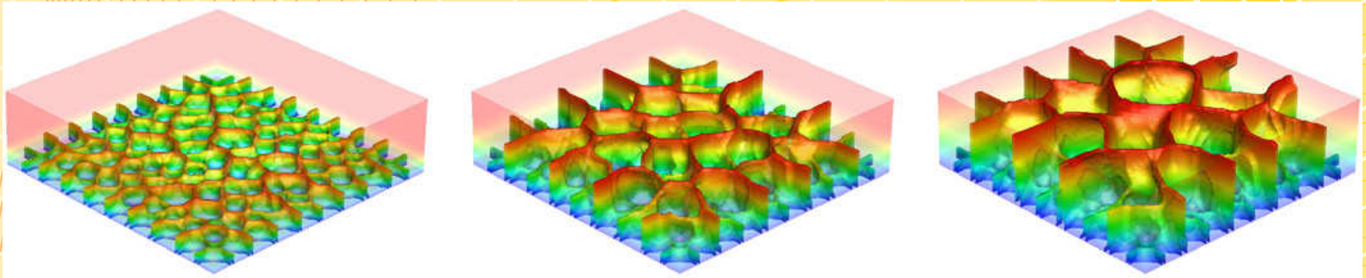

Figure 1: Phase-field simulation of drying soil (Miehe & Mauthe, Univ. Stuttgart)

Phase-field models are an important class of mathematical techniques for the description of a multitude of industry-relevant physical and technical processes. Examples are the modeling of cracks and fracture propagation in solid media like ceramics or dry soil (see Figure and [1]), the representation of liquid phase epitaxy [2] for solar cells, semi-conductors or LEDs as well as melting and solidification processes of alloys.

The price for the broad applicability and mathematical elegance of this approach is the significant computing cost required for the simulation of phase-field equations at large scales. Solutions of these equations typically contain sharp interfaces moving through the domain. Such structures can only be resolved with carefully tuned, adaptive discretization schemes in space and time. Even worse, many key phenomena start to emerge only when the simulation domain is large and the simulation time is long enough. For example, in order to simulate micro cracks leading to fatigue failure of a piece of machinery, the domain must contain a certain number of these cracks. For epitaxy, in turn, structures are normally described on nano-scales, while the specimen sizes are on the order of centimeters. Thus, the enormous number of degrees-of-freedom for the discretization in space and time as well as the significant complexity of the simulation demand the use of modern HPC architectures.

The goal of the BMBF project "ParaPhase - space-time parallel adaptive simulation of phase-field models on HPC architectures" (FKZ 01IH15005A, BMBF program "IKT 2020 - Forschung für Innovation") is the development of algorithms and methods that allow for highly efficient space-time parallel and adaptive simulations of phase-field problems. Three key aspects will be addressed in the course of the project:

1. Heterogeneous parallelization in space. The adaptive phase-field multigrid algorithm TNNMG [3] will be parallelized using load-balanced decomposition techniques and GPU-based acceleration of the smoother.
2. Innovative parallelization in time. For optimal parallel performance even on extreme scale platforms, novel approaches like Parareal and the "parallel full approximation scheme in space and time" [4] for the parallelization in the temporal direction will be used, exploiting the hierarchical structures of spatial discretization and solver.
3. High-order methods in space and time. To increase the arithmetic intensity, i.e., the ratio between computation and memory access, flexible high-order methods in space (using the Discontinuous Galerkin approach) and time (using spectral deferred corrections) will be implemented and combined.

This project brings together scientists from applications, numerical mathematics and HPC. The consortium is lead by JSC and consists of six German partners: Prof. Dr.-Ing. Heike Emmerich, Chair for Materials and Process Simulations at Universität Bayreuth, JProf. Dr. Carsten Gräser, Department of Mathematics and Computer Science at Freie Universität Berlin, Prof. Dr.-Ing. Christian Miehe, Chair of Material Theory at Universität Stuttgart, Prof. Dr. Oliver Sander, Institute of Numerical Mathematics at Technische Universität Dresden, Dr. Robert Speck, Jülich Supercomputing Centre at Forschungszentrum Jülich GmbH, and Jiri Kraus at NVIDIA GmbH.

With two partners with a long-standing experience in the particular field of applications (the groups of Heike Emmerich and Christian Miehe) as well as four partners with a strong background in methods, algorithms and HPC (the groups of Carsten Gräser, Oliver Sander, Robert Speck and Jiri Kraus), one of the key goals of this project is the mutual extension of competences: While the application scientists will ultimately be able to work with unprecedented resolutions in space and time on modern HPC platforms, the HPC experts and method developers will have the unique opportunity to test and tune their ideas for industry-relevant, highly complex problems. The algorithms developed in this project will be primarily used for studying fracture propagation and liquid phase epitaxy, but these problem classes already represent a wide range of challenges in industrial applications. Based on the open source software Dune, the "Distributed and Unified Numerics Environment" [5], the resulting algorithms will help to make large-scale HPC simulations accessible for researchers in these fields.

The Kickoff Meeting is planned for the end of May 2016, marking the official start of this three-years project. With two postdocs and three PhD students fully funded by BMBF, this will also contribute to the educational effort in the field of computational science and engineering, enabling young scientists to address challenges of real-world applications with HPC-ready methods and algorithms.

References

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Projects

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