Progress in Large-Scale Differential Variational Inequalities for Heterogeneous Materials

Large-Scale Differential Variational Inequalities for Heterogeneous Materials
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Abstract

This presentation will discuss the development of advanced numerical techniques and scalable software for differential variational inequalities (DVIs) for the resolution of large-scale, heterogeneous materials problems. Such problems describe the mesoscale behavior of irradiated materials and are of central interest to our partner Energy Frontier Research Center (EFRC), the *Center for Materials Science of Nuclear Fuel* (CMSNF), which has the mission of developing a computationally predictive, experimentally validated, multiscale understanding of the thermo-mechanical behavior of nuclear fuel. We will discuss three aspects of research: (1) modeling phase field equations as DVIs, (2) applying semismooth and active set methods using multigrid preconditioners to these models, and (3) developing scalable software for solving the resulting variational inequalities (VIs).

Mesoscale materials modeling is challenging because the evolution of each diffusive boundary between a void and the surrounding matrix must be correctly predicted. The CMSNF is using the phase field approach. Since the diffuse boundary between phases must be localized, one needs to use double obstacle potentials for generating the free energy functional. This results in a DVI. However, the lack of software for large-scale DVIs has led to the situation where the prevailing approach approximates the dynamics of the phase variable using a smoothed potential. In turn, this (non-DVI) method results in a stiff problem and undesirable physical artifacts: the phase field variable does not have a compact support, and the boundary between phases—grains in the case of irradiated materials—is no longer localized.

To circumvent these difficulties, we solve the problem in its natural formulation: the one of DVI, which is equivalent to a complementarity problem. This approach in turn allows us to use newly developed nonlinear algebraic VI solvers in PETSc: a semismooth algorithm and two projected gradient reduced-space active set algorithms, which leverage experience in TAO and PATH.

We employ coupled Cahn-Hilliard and Allen-Cahn systems with a double-obstacle free-energy potential to simulate the physics. Preliminary numerical experiments and mathematical analysis for both the Allen-Cahn and Cahn-Hilliard systems, as well as coupled systems, demonstrate mesh-independent convergence rates for multigrid-based preconditioners. That is, the work required to solve a single timestep grows linearly with the number of unknowns. We have validated the DVI approach against the baseline results of the CMSNF; we employed much larger time steps than conventional methods, which is one of the projected benefits of the DVI formulation. We are extending to address multigrain and void simulations as needed by the CMSNF.

Our approach is well suited to leverage emerging extreme-scale computing resources for scientific discovery by incorporating billions of discretization nodes. The result will be the ability to simulate thousands of grains and thus develop a predictive capability for virtually any phenomenon of interest concerning radiation in nanostructures. Moreover, these new algorithms and software have broader applicability to additional DOE simulations that can employ DVIs to overcome difficulties in modeling phase changes, free boundaries, and hybrid discrete-continuum behavior.