11-3056: Multiscale Modeling and Uncertainty Quantification for Nuclear Fuel Performance

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ABSTRACT

Developing sustainable nuclear fuel cycles is a principal priority of the Office of Nuclear Energy in the Department of Energy. The use of model simulations of fuel behavior can be a cost-effective means to accelerate development by reducing the need for prototypes and large-scale experiments. But, model simulations must undergo a rigorous process of validation and uncertainty quantification in order to assess their predictive capability. This is a difficult undertaking. As energy is converted into heat in the fission process, there are significant microstructure and composition changes in the fuel that affect the chemical, thermal and mechanical properties of fuels. Predictive simulation of nuclear fuel forms must account for these changes.

Existing fuel performance models are mostly semi-empirical and are calibrated by materials data collected under a wide range of conditions. This leads to significant limitations in terms of predicting behavior in the dynamic environment in nuclear reactors. This has motivated new efforts to develop high-fidelity models of nuclear fuels that are multiscale in nature, and integrate the fundamental radiation damage and defect behavior at the crystal lattice level into the continuum (engineering) scale via sophisticated mesoscale models of microstructure evolution in irradiated fuel.

Multiscale models raise a number of significant challenges. Both developing high fidelity models for each scale and formulating coupling methods between models at different scales that yield high fidelity behavior are difficult problems. Multiscale models are complex nonlinear systems with complicated dynamical behavior and computing accurate numerical solutions is another difficult challenge. Another significant complication for modeling fuel performance is that any model is inherently stochastic because of experimental error, modeling error, and the statistical nature of some components. The consequence is that multiscale modeling of nuclear fuel performance is computationally intensive undertaking.

In this project, we will address the challenges associated with constructing high fidelity multiscale models of nuclear fuel performance. We propose a novel approach for coupling mesoscale and macroscale models, devise efficient numerical methods for simulating the coupled system, and devise and analyze effective numerical approaches for error and uncertainty quantification for the coupled multiscale system. As an integral part of the project, we will carry out analysis of the effects of upscaling and downscaling, investigate efficient methods for stochastic sensitivity analysis of the individual macroscale and mesoscale models, and carry out a posteriori error analysis for computed results. While we pursue development of the methodology in the context of a particular multiscale model of interest to the Idaho National Laboratory and, more broadly, to the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program, our techniques will apply to a wide class of multiscale models for nuclear fuel performance.