Predictive Maturity of Multi-Scale Simulation Models for Fuel Performance

PI: Sez Atamturktur – Clemson University

Program: FCR&D

Collaborators: Brian Williams, Cetin Unal, Francois Hemez & Carlos Tome – Los Alamos National Laboratory

ABSTRACT

The focus of nuclear fuel design and maintenance has been shifting from a primarily empirical endeavor to the use of highly advanced simulations with experiment-based validation and uncertainty quantification. For the Office of Nuclear Energy (NE) to address the nation's energy needs, assessment of the *predictive maturity* of these simulation models is essential. Herein, Predictive maturity refers to the degree of confidence that decision-makers can place in a simulation. For a program governed by advanced simulation tools to be successful, the development of procedures that quantify the predictive maturity of multi-scale multi-physics nuclear reactor simulations must supplement NE's code development and experimental efforts.

This project proposes to provide a predictive maturity framework with its companion metrics that (1) introduce a formalized, quantitative means to communicate information between interested parties, (2) provide scientifically dependable means to claim completion of validation and uncertainty quantification (VU) activities, and (3) guide the decision makers in the allocation of NE's resources for code development and physical experiments.

The project team proposes to develop this framework based on two complimentary criteria: (1) the extent of experimental evidence available for the calibration of the simulation model and (2) the sophistication of the physics incorporated in the simulation model. The proposed framework will be capable of quantifying the interaction between the required number of physical experiments and degree of physics sophistication. Because making an objective statement about the sophistication of a simulation model is extremely difficult, sophistication will be defined in relative terms—i.e., coupling atomistic-level simulation results with continuum performance simulations is expected to increase the sophistication of the higher-level simulations.

A practical application of the proposed framework will be illustrated using a mesoscale polycrystal plasticity code for modeling creep of core reactor clad and duct components subjected to in-service conditions of irradiation, stress, and thermal cycling. Using a layered approach, the project team will first improve the physics model by coupling two distinct atomistic scale simulations with the mesoscale model. This coupling will produce a multi-scale model that will incorporate information from: (1) atomistic simulations of configurations and diffusivity of vacancies and interstitials, and (2) atomistic simulations of dislocation-loop and dislocation-bubble interactions. This work will yield several versions of the polycrystal plasticity code of varying levels of physics complexity. Then, we will calibrate the multiple versions of the multi-scale model against varying amounts of experimental information. For calibration, both in-reactor creep experiments of pressurized mini-tubes and ex-situ creep experiments of pre-irradiated material will be used. Experimental uncertainty will be incorporated in the analysis. The predictive maturity framework will be applied to investigate the fidelity and uncertainty of the multi-scale simulation code as increasing amounts of physical experiments and first-principle physics are incorporated. A fundamental component of the predictive maturity framework is the active process of identifying the next stages of improvement. Therefore, the outcomes of this project will identify the most beneficial future directions in code development and experimentation for the polycrystal plasticity model to maximize the gain in predictive maturity.