Phenomena-based Uncertainty Quantification in Predictive Coupled-Physics Reactor Simulations

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ABSTRACT

This project seeks to develop methodologies, tailored to the physical phenomena that govern nuclear-reactor behavior, to produce predictions (including uncertainties) for quantities of interest (QOIs) in the simulation of steady-state and transient reactor behavior. Such predictions include, for each QOI, not only the expected value but also a distribution around this value and an assessment of how much of the distribution stems from each major source of uncertainty. The project will test its methodologies by comparing blind predictions against measured experimental outcomes. While reactor transients with strong feedback are inherently complex, we have devised a setting that permits generation of substantial validation-quality data and offers the prospect of reasonable quantitative estimates of uncertainties in predicted QOIs.

Producing predictive distributions with quantified, traceable uncertainties is an important unsolved problem across a broad spectrum of computational science and engineering applications, including many applications relevant to nuclear energy. If computational simulations cannot produce such distributions (or equivalent output that conveys the same key information), their value to decision-making is limited. This project aims to help solve this problem and thereby boost the value of simulation for a number of DOE/NE programs.

In particular, the project addresses several important outstanding problems in predictive science and engineering. One is the problem of introducing physics into statistical models that attempt to account for uncertainties. Another is the problem of high-dimensional inputparameter spaces. We attempt to address both of these via our physics-based model for a correction to a cross section that is known to be approximate. Calibration of all of the numbers in a temperature-dependent multigroup scattering cross section would be intractable; our parameterization of a Gaussian pairwise distribution function is a form of physics-based dimension reduction that addresses this. A third important problem is how to infer information about one phenomenon in the presence of a "background" of other phenomena, which may introduce uncertainties that drown out the information that is sought. In our case the "signal" that we seek is the sensitivity of reaction rates to the details of the bound-H inelastic scattering model and the "noise" is the set of uncertainties from other cross sections, from discretization error, and from other physical phenomena.