

– Poster –

High Performance Embedded Hybrid Methodology for Uncertainty Quantification in Multi-physics Problems

A. Mittal, G. Iaccarino (Stanford University), B. Lee (PNNL), C. Tong (LLNL)

Abstract

In this poster we present the formulations of a new computational framework for high-performance UQ analysis of large-scale multi-physics systems based on a hybrid approach, which uses a blending of intrusive and non-intrusive methods in a computational model, and illustrate some simple examples. More specifically, this framework emphasizes a sound mathematical analysis and high parallel efficiency to propagate uncertain variables through the various physics modules. The proposed hybrid approach seeks to overcome the difficulties with both intrusive and non-intrusive approaches by incorporating UQ methods best suited or only available for each individual physics module, and seamlessly gluing these modules together to facilitate uncertainty propagation and data fusion for the full system.

The hybrid methodology adopts a divide-and-conquer approach to quantifying uncertainties in a complex system. To successfully develop this methodology, a deterministic multi-physics model is first partitioned into modules with simpler physics, in a similar fashion to the operator splitting partitioning often performed on modern simulation codes. Next, each module is equipped with the best UQ methods available to it. But in order to couple the modules and propagate uncertainties correctly and efficiently through the full system, several challenges must be addressed. These challenges include, (1) how to propagate uncertainties given that each module may employ a different UQ method and thus have different uncertainty representations, (2) how to exploit the modular structure of the problem to efficiently tackle high-dimensional (large number of uncertain parameters) models, (3) how to perform Bayesian data fusion in a hybrid framework, and (4) how to tune the components of the hybrid method to achieve good performance on future extreme scale computers.

In the first phase of the project we addressed the first two items. We currently adopt a polynomial chaos expansion (PCE) for the system output at the full system level; software wrappers *package* the uncertainties in various ways depending on the intrinsic UQ methodology available within each specific physics module. We have demonstrated the use of the wrappers in a coupled problem in which two modules with different embedded UQ methods are present. The results are encouraging and show that it is indeed possible to hide the details of the full-system UQ problem from the module-specific implementation. From a computational perspective the accuracy and convergence of the present approach has been investigated and initial results will be reported.

Current activities are focused on the identification of the mathematical framework that allows us to analyze the flow of uncertainties, characterizes the coupling between modules, and extracts structures embedded in the physics in order to guide adaptive dimension reduction for accelerating uncertainty propagation. The long term objective is to apply the hybrid methodology on three challenging multi-physics applications: coupled neutronics/thermal-hydraulics in a nuclear reactor core, subsurface reservoir modeling and coupled flow/thermal transport in extreme environmental conditions.