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Uncertainty Quantification in Computational Models



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Dr. Najm's research has spanned development of numerical methods for reacting flow computations, computational studies of laminar flames with detailed chemical kinetics, development of UQ methods and their application in reacting flow, analysis and reduction of multiscale chemical systems, modeling of electrochemical microfluid systems, statistical data analysis for biodetection, stochastic dynamical systems, and Bayesian inference methods for inverse problems. He serves on the editorial board of the *International Journal for Uncertainty Quantification* and is the author/co-author of more than 80 journal articles. He holds 11 U.S. patents.

The estimation of uncertainty in inputs and outputs of computational models is critical for achieving truly predictive computations of physical systems. At Sandia, years of research about uncertainty quantification (UQ) algorithms for both inverse and forward problems has resulted in their implementation in open-source software, including both the UQTk and Dakota libraries. These tools have aided UQ studies in computational modeling of a range of physical systems, including chemical kinetic modeling of hydrocarbon fuels, fluid flow, climate modeling, power grids, and fusion systems. Currently, these capabilities are being applied to Large Eddy Simulation of turbulent supersonic multiphase combustion in a SCRAMJET engine.

In his talk, Dr. Najm will discuss some recent UQ developments, including the statistical estimation of model error, useful for assessment of meaningful predictive uncertainties and for diagnostic purposes in model development. He will include using multi-level, multi-fidelity methods in the context of both global sensitivity analysis and forward UQ that address the challenge of high dimensionality and computational complexity. He will illustrate using these capabilities in the context of targeted model problems, as well as in computations of the jet-in-crossflow SCRAMJET engine subsystem.



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