Multidisciplinary Simulation, Estimation, and Assimilation Systems

Joint MSEAS and Reacting Gas Dynamics Lab Seminar

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Uncertainty Quantification in Computational Models

Abstract: Models of physical systems generally involve inputs and/or parameters that are determined from empirical measurements, and therefore exhibit a certain degree of uncertainty. Estimating the propagation of this uncertainty into computational model output predictions is crucial for purposes of model validation, design optimization, and decision support.

Recent years have seen significant developments in probabilistic methods and tools for efficient uncertainty quantification (UQ) in computational models. These tools are grounded in the use of Polynomial Chaos (PC) expansions for representation of random variables. The utility and effectiveness of PC methods have been demonstrated in a range of physical models, including structural mechanics, transport in porous media, fluid dynamics, aeronautics, heat transfer, and chemically reacting flow. While high-dimensionality remains nominally an ongoing challenge, great strides have been made in dealing with moderate dimensionality along with non-linearity and oscillatory dynamics.

In this talk, I will give an overview of UQ in computational models, with a focus on chemical systems. I will cover both halves of the UQ problem, namely: (1) the estimation of uncertain input parameters from empirical data, and (2) the forward propagation of parametric uncertainty to model outputs. I will cover the basics of forward PC UQ methods with examples of their use. I will also highlight the need for accurate estimation of the joint probability density over the uncertain parameters, in order to arrive at meaningful estimates of model output uncertainties. Moreover, I will discuss novel methods for estimating this density given partial information from legacy experiments, in the absence of raw data.

Friday, Oct. 14, 2011

1:00PM; Rm. 5-314

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