



## NNSA PRISM Seminar Series – Fall 2008



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### ***Uncertainty Quantification in Chemical Systems***

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3:00pm  
Birck 1001

**Abstract:** Uncertainty quantification in computational modeling is important for both engineering design and model validation. We have employed spectral stochastic techniques for uncertainty quantification in the modeling of chemical systems, where uncertain quantities are modeled stochastically, and are represented using polynomial chaos expansions (PCEs). I will discuss the utility of these constructions in chemically reacting flow computations, including both sampling-based non-intrusive implementations and direct methods based on Galerkin projection of the governing equations. I will also discuss challenges faced using conventional Wiener-Hermite PCEs in chemical systems, and outline the resolution of these challenges using PCEs with multiwavelet constructions employing local bases on block-decomposed stochastic space. Finally, I will highlight the important role of correlations among uncertain parameters, and the consequences of strong non-linearity and fast time scales in chemical systems.



**Bio:** Habib N. Najm is a Distinguished Member of the Technical Staff at Sandia National Laboratories in Livermore, CA. He received the MS and PhD degrees in Mechanical Engineering from the Massachusetts Institute of Technology in 1986 and 1989, and the BE degree in Mechanical Engineering from the American University of Beirut in 1983. Before joining Sandia in 1993, Dr. Najm worked with Texas Instruments on advanced measurement techniques for semiconductor processing, and on studies of thermofluid systems in semiconductor process technology. His work at the Sandia Combustion Research Facility covers a range of computational reacting flow research, with a focus on the development and utilization of advanced algorithms and software for computational studies of reacting flow with detailed chemical kinetics. He also works on the development of stochastic numerical methods for uncertainty quantification in thermofluid systems; on computational studies of stochastic dynamical systems and electrochemical microfluid systems; and on Bayesian statistics techniques for inverse problems and for analyte classification in micro/nano-channel biotechnology devices. Dr. Najm is co-author of over fifty archival journal articles and 11 US patents.

Refreshments will be served. For further information please contact Prof. Dongbin Xiu at: [dxiu@math.purdue.edu](mailto:dxiu@math.purdue.edu)  
For information about PRISM visit: <http://www.purdue.edu/discoverypark/prism/>  
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