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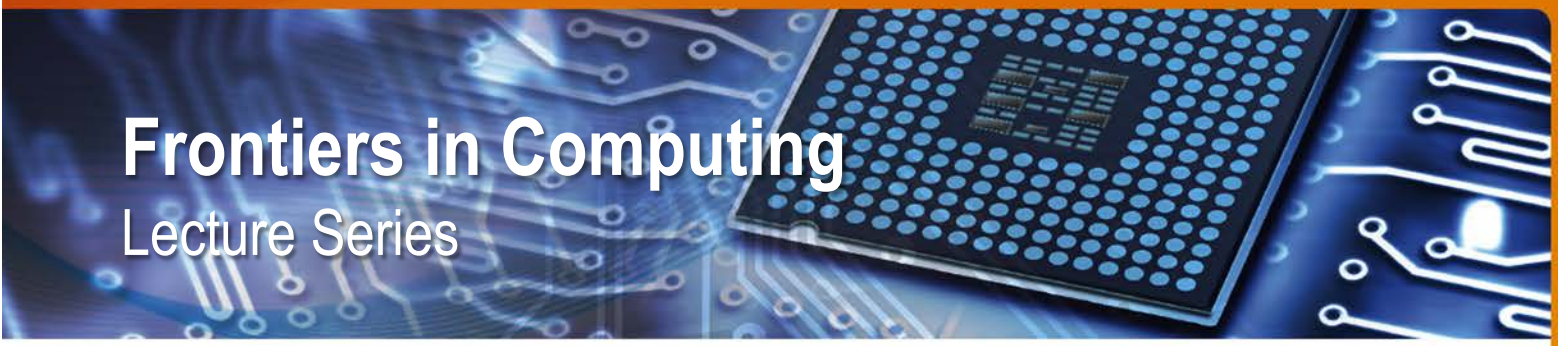

Frontiers in Computing
Lecture Series

Uncertainty Quantification in Multiscale Simulations

Nicholas Zabaras, Ph.D.

Viola D. Hank Professor of Computational Science and Engineering, University of Notre Dame

Friday, February 10, 2017
10 AM ◆ ISB2/Wanapum (155)

Professor Zabaras' research focuses on the integration of computational mathematics, statistics, and scientific computing toward predictive modeling of complex system. He has been honored with the Wolfson Research Merit Award from the Royal Society, the Michael Tien '72 Excellence in Teaching Prize from Cornell University, and the Presidential Young Investigator Award from the National Science Foundation. He serves as Editor in Chief of the *International Journal for Uncertainty Quantification* and Associate Editor of the *Journal of Computational Physics* and *Communications in Computational Physics*. He joined Notre Dame after serving as the founding director of the Warwick Centre for Predictive Modeling at the University of Warwick. He currently serves as Hans Fisher Senior Fellow at the Institute for Advanced Study at the Technical University of Munich. He spent 23 years in all academic faculty ranks within the Sibley School of Mechanical and Aerospace Engineering at Cornell, where he was the director of the Materials Process Design and Control Laboratory. He also received his Ph.D. in Theoretical and Applied Mechanics from Cornell.

The high stochastic dimensionality, multiscale/multiresolution/multiphysics, and often phenomenological nature of models in science and engineering provide many unique mathematical challenges in the context of uncertainty quantification, predictive modeling, and design under uncertainty. With his talk, Dr. Zabaras will address two unifying themes typical of multiscale simulations using materials physics as the application domain: 1) the use of surrogate models and 2) stochastic coarse graining (CG). He will advocate data-driven machine learning approaches for both challenges. Part of his talk will center on a Bayesian framework for alloy modeling using the cluster expansion, where he will show the framework's performance in predicting various thermodynamic properties. He also will discuss and present an assessment of a data-driven, CG atomistic formulation in the context of equilibrium statistical mechanics. In contrast to existing CG techniques based on a fine-to-coarse map, it engages an opposite strategy by prescribing a generative probabilistic coarse-to-fine map that quantifies the uncertainty.

Host: Nathan Baker (nathan.baker@pnnl.gov), ACMD Division Director

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