Abstract: Predictive modeling of physical processes in heterogeneous materials requires innovations in mathematical and computational thinking. While recent multiscale approaches have been successful in modeling the effects of microstructure to macroscopic response, a significant grand challenge remains in understanding the effects of microstructural and other uncertainties in characterization of properties and in the design of heterogeneous materials. To address these problems, we are developing a mathematical framework that provides a paradigm shift in the predictive modeling of complex systems in the presence of uncertainties in order to address major limitations in modeling stochastic PDEs: (i) The stochastic inputs are mostly based on ad hoc models, (ii) The number of independent stochastic parameters is typically very high, and (iii) Deterministic simulations of physical processes in heterogeneous media are expensive.

To address issue (i), we are developing non-linear data-driven model reduction strategies. To address issues (ii) and (iii), we are developing low-complexity surrogate models of the high-dimensional stochastic multiscale system under consideration. In this presentation, we will briefly discuss recent work towards the development of an efficient, Bayesian Uncertainty Quantification (UQ) framework using a novel treed Gaussian process model. While traditional UQ methods build a surrogate of the computer code, our framework results in a probability distribution over the possible surrogates, effectively quantifying the epistemic uncertainty introduced by the finite number of simulations. Furthermore, the scheme explicitly models correlations between discrete outputs of the code as well as in space and time.

Finally, a number of examples will be discussed in the data-driven representation of random heterogeneous media and in modeling physical processes (multiscale deformation, thermal/hydrodynamic transport, etc.) in such media.

Biography: After completing doctoral work in Theoretical and Applied Mechanics, Professor Zabaras joined the faculty of the Mechanical Engineering Department at the University of Minnesota, Minneapolis, MN. He became a Cornell faculty member in 1991. Zabaras is a Fellow of the American Society of Mechanical Engineers, and member of the American Physical Society, the American Academy of Mechanics, the Society for Industrial and Applied Mathematics and the Minerals, Metals & Materials Society. He received a Presidential Young Investigator Award from the National Science Foundation in 1991.

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