Uncertainty Quantification and Predictive Modeling in Heterogeneous Media and Polycrystalline Materials

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Abstract

Predictive modeling of physical processes in heterogeneous media and in particular in polycrystalline 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 microstructure and other uncertainties in characterization of properties and in materials design. We will address two major issues: (i) Developing reduced-order stochastic models of the microstructure input uncertainty and (ii) techniques to account for the large stochastic dimensionality in the solution of the underlying physical problems. To address the former, we are developing various non-linear data-driven model reduction strategies. To address the latter, we will discuss low-complexity surrogate models of the high-dimensional stochastic multiscale system under consideration. We will touch upon ideas based on manifold learning, kernel PCA, locally weighted projection regression methods, sparse Bayesian kernel techniques, adaptive sparse grids and HDMR and others.

A number of examples will be introduced in modeling physical processes (deformation, thermal/hydrodynamic transport, etc.) in random media and polycrystals. They include calculation of probabilistic distributions of properties of multi-phase alloys including elastic properties, strength, and fatigue properties. Convex hulls of all possible anticipated properties and the corresponding probabilities in the presence of microstructure uncertainties will be shown.

We will finally address predictive multiscale modeling of polycrystalline materials and provide potential mathematical and statistical avenues for resolving the underlying issues of complexity and curse of dimensionality within an information theoretic framework.

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