Uncertainty Quantification and Predictive Multiscale Materials Modeling

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Abstract

We will briefly review several areas of uncertainty quantification and their relevance to predictive materials science. At first, we will discuss solution of stochastic differential equations using recently developed efficient Bayesian approaches (Gaussian processes, relevance vector machines, etc.). We will then introduce microstructure probabilistic model reduction algorithms using manifold learning and Bayesian approaches. An efficient scheme for simultaneous microstructure model reduction on both mesoscale and macroscale (biorthogonal KLE decomposition) will be presented. We will integrate these techniques to address stochastic multiscale modeling of polycrystalline materials (e.g. computing fatigue properties of superalloys). We will also discuss a framework for posing such stochastic multiscale materials problems as inference problems using probabilistic graphical models. We will finish with discussion of open problems and potential impact of this work.