Modeling and Simulation of High Dimensional Stochastic Multiscale PDE Systems at the Exascale

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Abstract

We will discuss uncertainty quantification for fluid transport in heterogeneous media in the presence of both stochastic permeability and multiple scales. A new mixed multiscale finite element method is first developed within the framework of the heterogeneous multiscale method (HMM) in the spatial domain. It ensures both local and global mass conservation. Starting from a specified covariance function, the stochastic log-permeability is discretized in the stochastic space using a truncated Karhunen-Loève expansion with several random variables. Due to the small correlation length of the covariance function, this often results in a high stochastic dimensionality. To deal with the computational cost of such simulations, we introduce kernel principal component analysis for stochastic input model generation to reduce the dimensionality of the permeability field and generate realizations with similar spatial statistical attributes. Through use of kernel functions, KPCA enables the preservation of higher-order statistics of the random field, instead of just two-point statistics. Thus, this method can model non-Gaussian, non-stationary random fields. A new approach to solve the pre-image problem involved in KPCA is introduced. In addition, polynomial chaos (PC) expansion is used to represent the random coefficients in KPCA which leads to a parametric stochastic input model. Thus, realizations, which are statistically consistent with the experimental data, can be generated in an efficient way. Uncertainty quantification is performed by sampling directly in the reduced-order surrogate input space. We demonstrate this framework using data of heterogeneous channelized permeability and calculating the statistics of the flow. We will present uncertainty propagation applications using the high dimensional model representation technique (HDMR) where the component functions are computed with adaptive sparse grids, using multi-level Monte Carlo method and a newly developed Bayesian uncertainty quantification approach based on Gaussian processes.