Modeling diffusion in random heterogeneous media: Data-driven microstructure reconstruction models, stochastic collocation and the variational multiscale method[1]

Nicholas Zabaras and Baskar Ganapathysubramanian
Materials Process Design and Control Laboratory
Sibley School of Mechanical and Aerospace Engineering
188 Frank H T Rhodes Hall
Cornell University
Ithaca, NY 14853-3801

We are interested in modeling diffusion in 3D random heterogeneous microstructures that are defined through limited statistical information extracted from 2D microstructure snapshots. An accurate simulation of diffusion in random heterogeneous media has to satisfactorily account for the twin issues of randomness as well as the multi-length scale variations in the material properties. We propose a general methodology to construct a data-driven, reduced-order microstructure representation model to describe property variations in realistic heterogeneous media. This reduced-order model then serves as the input to the SPDE describing thermal diffusion through random heterogeneous media. A decoupled scheme is used to tackle the problems of stochasticity and multi-length scale variations in properties. A sparse-grid collocation strategy is utilized to reduce the solution of the SPDE to a set of deterministic problems. A variational multiscale method with explicit subgrid modeling is used to solve these deterministic problems. An illustrative example using experimental data is provided to showcase the effectiveness of the proposed methodology.

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