Advances in numerical methods for stochastic partial differential equations and stochastic homogenization

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Introduction. Many applications include inherent stochasticity and thus require modeling by stochastic partial differential equations. Associated multiscale problems lead to problems in the numerical stochastic homogenization of PDEs. Numerical problems arising from stochastic PDEs are at the core of uncertainty quantification and are usually very computationally expensive due to the usually large number of stochastic dimensions.

We present various results by our group from the development of new methods for this type of problems. Concrete applications for which numerical results are presented include functional devices in nanotechnology such as nanoscale sensors, where we develop new simulation capabilities in order to enable their rational design.

Numerical methods. We present the first multi-level Monte-Carlo algorithm for a system of stochastic PDEs, namely for the stochastic drift-diffusion-Poisson system. This system is fundamental for charge transport through random environments. The error estimate is discussed as well as the optimal choice of the number of evaluations at each level and the refinement between the levels in a multi-level MC approach. These considerations yield the optimal multi-level MC algorithm.

The second set of results concerns the numerical stochastic homogenization of elliptic equations. We consider binary materials with random inclusions, thus exhibiting a random microscopic structure described by a piecewise constant, stochastic coefficient in the elliptic operator. Then the mechanical properties of the material are essentially described by elliptic equations for each component of a tensor. We present Monte-Carlo, quasi Monte-Carlo, and multi-level Monte-Carlo algorithms for calculating the effective coefficient.

The third set of results describe a basis-adaptation approach for elliptic problems, where the quantity of interest is a nonlinear functional of the solution. It is found that significant speed-ups are possible for a certain choice of basis functions.

Numerical results. We present simulation results for concrete applications. We apply the numerical methods above to charge transport through a random environment in order to quantify process variations. We also calculate inherent noise and fluctuations in nanoscale sensors in order to quantify their signal-to-noise ratio and detection limit. Finally, the numerical homogenization results allow us to design the macroscopic properties of materials with a random microscopic structure. The numerical methods above are essential for modeling and simulation based on stochastic PDEs, since the computational cost would be prohibitive otherwise.

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