Optimal Numerical Methods for Stochastic Homogenization and the Stochastic Drift-Diffusion-Poisson System

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Introduction. Numerical stochastic homogenization and the numerical solution of stochastic partial differential equations are computationally very demanding, since the evaluation of a single sample requires solving a partial differential equation. When developing numerical algorithms for these kinds of problems, there are usually parameter values in the discretizations such as the fineness of a finite-element discretization and the number of samples in each level of a multi-level approach that need to be determined in rational manner.

The numerical problems. We consider two leading examples. The first is the numerical stochastic homogenization of elliptic problems, and in particular the case where the permittivity or diffusion constant is piecewise constant for modeling the physical situation of randomly distributed inclusions in a background material.
The second problem is the solution of the drift-diffusion-Poisson system with all stochastic coefficients for modeling charge transport in random environments. Real-world applications are the effect of random dopants in nanoscale transistors or the simulation of nanoscale field-effect sensors.
For both of these problems, we have been developing algorithms that minimize the computational work for a given prescribed total error [1, 2, 3]. The basic idea is to find estimates for the total error (using as few inequalities as possible) and to model the computational work as a function of the unknown discretization parameters. Then the optimal discretization parameters are found as the solution of a nonlinear optimization problem, whose coefficients modeling the computational work have been measured.

Results and Discussion. We present results from applying these ideas to the two model problems mentioned above. In the case of the numerical stochastic homogenization of elliptic problems, an optimal algorithm was developed in [1], and improvements will be reported here.
Regarding the stochastic drift-diffusion-Poisson system, an optimal multi-level approach was developed in [2]. It was found that the computational work can be reduced by orders of magnitude compared to the standard Monte-Carlo method, and the reduction increases as the prescribed total error decreases. More recently, we have developed a randomized quasi Monte-Carlo extension [3] of the previous work [2].
In all cases, we discuss the error estimates used, the modeling and measurement of the computational work, the resulting optimization problems, and we show numerical results in order to assess the improvements.

Références

[1] Caroline Geiersbach, Clemens Heitzinger, and Gerhard Tulzer, *Optimal approximation of the first-order corrector in multiscale stochastic elliptic PDE*, SIAM/ASA J. Uncertainty Quantification, 4(1):1246–1262, 2016. DOI: 10.1137/16M106011X.

[2] Leila Taghizadeh, Amirreza Khodadadian, and Clemens Heitzinger, *The optimal multilevel Monte-Carlo approximation of the stochastic drift-diffusion-Poisson system*, Computer Methods in Applied Mechanics and Engineering (CMAME), 318:739–761, 2017. DOI: 10.1016/j.cma.2017.02.014.

[3] Leila Taghizadeh, Amirreza Khodadadian, and Clemens Heitzinger, *Optimal multi-level randomized quasi Monte-Carlo method for the stochastic drift-diffusion-Poisson system*, *in preparation.*

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