Toward Exascale Computations of Uncertainty Quantification for Porous Media Flow Using Multilevel Monte Carlo

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Uncertainty quantification (UQ) for porous media flow is of great importance for many societal, environmental and industrial problems. An obstacle to the progress in solving such problems, as well as in solving other stochastic PDEs, SPDEs, is the extreme computational effort needed for solving realistic problems. It is expected that the computers will open the door for a significant progress in this area. We shortly introduce the Distributed and Unified Numerics Environment DUNE [www.dune-project.org], and demonstrate how new features, developed in the last few years, can enable the handling of these computational challenges. In the frame of the DFG funded project EXA-DUNE, the software has been extended by multiscale finite element methods (MsFEM) and by a parallel framework for the multilevel Monte Carlo approach (MLMC). This is a general concept for computing expected values of simulation results depending on random fields, e.g. the permeability of porous media. It belongs to the class of variance reduction methods and overcomes the slow convergence of classical Monte Carlo by combining cheap/inexact and expensive/accurate solutions in an optimal ratio.

Let us discuss shortly different components of the considered algorithm and its implementation.

Different approaches have been developed for solving stochastic PDE. Perturbation methods, moment equations, generalized polynomial chaos and various Monte Carlo methods have been extensively studied. Our choice is an efficient variant of the

Monte Carlo methods, namely Multilevel Monte Carlo method.As mentioned above, the idea of this method is to reduce variance by combining cheap/inexact and expensive/accurate solutions in an optimal ratio. Selection of the levels in MLMC is an open question and is subject of intensive research. For example, if one uses Karhunen-Loewe expansion to reduce the dimensionality in the stochastic space, the number of the terms in the expansion can be used to define levels in MLMC. Another approach for selecting levels in MLMC can be the number of the basis functions if reduced basis method is used. A more classical approach is to define levels by considering fine and coarsened grids. In the latter case when has to define the permeability on the coarse grid. In our talk we will elaborate on this last approach and will show results when renormalization is used to define the permeability on the coarser grids.

Another component of the algorithm is the generation of the permeability fields. This by itself is also a challenging computational task. Earlier we have reported on using circulant embedding for this purpose, and in this talk we will shortly recall those results.

For each realization of the permeability field one gets a deterministic PDE with highly varying coefficients which has to be solved efficiently. To discretize this PDE we use two methods: FEM and FV. In both cases we exploit DUNE software, www.dune-project.org. In the case of FEM discretization, also Multiscale FEM, MsFEM, can be used, and MsFEM solution can also be used to define levels in MLMC. We will recall some results on this approach.

Finally, the software implementation also plays essential role in solving stochastic PDE. High performance computing is demanded for solving such problems. We will shortly discuss the parallelization approaches implemented in DUNE, and will show results from the tests performed on the cluster in Fraunhofer ITWM. Currently only CPUs are used in our computations. In parallel, partners are working on parallelizing DUNE for heterogeneous architectures, and a goal of our future work is to have efficient implementation of MLMC on heterogeneous architectures. In particular, we plan to use MLMC also for coarse grain parallelization of algorithms for solving SPDE on exascale computers.

References

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