Multilevel Monte Carlo Method for Safety Analysis of Radioactive Waste Repositories

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Introduction

Safety of a deep radioactive waste repository is determined mainly by the permeability of the ground rock. In particular the residence time of radionuclides in the granite is especially sensitive to the position and connectivity of the fracture zones. Due to lack of the data there is usually a big uncertainty about the permeability, the location of the fracture, and other parameters of the rock. Therefore it is natural to consider these parameters as well as the results of a simulation to be random variables. For the safety analysis we are especially interested in the distribution function and quantiles of the concentration of radioisotopes either in a particular space-time point or as a space-time integral.

In order to capture preferential transport paths in the granite rock we consider a model of a Darcy flow and solute transport involving the coupling between a discrete fracture network of fractures and a continuum based on the concept due to Martin at al. [1]. In particular we have been developing Flow123d - a simulator of transport processes in fractured porous media [2].

Multilevel Monte Carlo method

Basic Monte Carlo method estimates a mean of a variable X (e.g. concentration) by the average $\overline{X}$ using N samples (simulations). This is attractive as it does not require changes in the simulation software. On the other hand the slow convergence of the variance (i.e. error) of the estimate:

$$\mathbf{D}\overline{X} \approx N^{-1/2}\,\mathbf{D}X$$

with respect to N prevents usage of this approach for realistic simulations.

The idea of multilevel Monte Carlo method (MLMC, see [3]) is to diminish the error of the mean estimate $\overline{X}$ not by increasing N but by reduction of the variable's variance $\mathbf{D}X$ by a sequence of approximations X^n that are cheaper to calculate. For appropriate problems one needs to run only few detailed simulations and large number of raw simulations with the total cost corresponding to the cost of the detailed simulations.

Approximation of the distribution function

MLMC is directly applicable to the approximation of the mean. To obtain an estimate for the distribution of a variable X we approximate its density function $\rho(x)$ using a suitable set I of general moments $\mathbf{E}\,\phi_i(X)$. In particular we use density approximation

$$\tilde{\rho}(x) = \exp\{-\sum_i \lambda_i \phi_i(x)\}$$

which matches the estimated moments $\mu_i = \overline{\phi_i(X)}$ and maximize the entropy:

$$\text{for} \quad \int_{-\infty}^{\infty} \phi_i(x)\tilde{\rho}(x)\,\mathrm{d}x = \mu_i \quad \text{for } i \in I$$

$$\text{maximize} \quad -\int_{-\infty}^{\infty} \tilde{\rho}(x)\ln(\tilde{\rho}(x))\,\mathrm{d}x.$$

The distribution function and quantiles are then calculated from the density approximation. Alternatively, we can approximate values of the distribution function $F(x) = \mathbf{E}\,H(X - x)$ by a smooth approximation of the Heaviside function $H(x)$.

Conclusion

We shall apply general (and well known) methods, in particular MLMC, described above to realistic 2D and 3D transport problems in a fractured porous media. In particular we use models with continuum-fracture coupling and explicit description of fracture network. We consider random permeability of the matrix and the fractures and randomly generated fracture network. We shall provide comparison of different approaches to the approximation of distribution functions and quantiles of the concentration using efficient MLMC calculations.

References

[1] Martin et al. *Modeling Fractures and Barriers as Interfaces for Flow in Porous Media*, SIAM Journal on Scientific Computing 26, no. 5 (2005).

[2] Brezina et al., Flow123d, URL: http://flow123d.github.com, (2011 – 2017)

[3] M. B. Giles. *Multilevel Monte Carlo methods*, Acta Numerica, 24, 259-328, (2015).