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## **Geostatistical Sampling Methods for Efficient Uncertainty Analysis in Flow and Transport Problems**

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In hydrogeological applications involving flow and transport of in heterogeneous porous media the spatial distribution of hydraulic conductivity is often parameterized in terms of a lognormal random field based on a histogram and variogram model inferred from data and/or synthesized from relevant knowledge. Realizations of simulated conductivity fields are then generated using geostatistical simulation involving simple random (SR) sampling and are subsequently used as inputs to physically-based simulators of flow and transport in a Monte Carlo framework for evaluating the uncertainty in the spatial distribution of solute concentration due to the uncertainty in the spatial distribution of hydraulic conductivity [1]. Realistic uncertainty analysis, however, calls for a large number of simulated concentration fields; hence, can become expensive in terms of both time and computer re-sources. A more efficient alternative to SR sampling is Latin hypercube (LH) sampling, a special case of stratified random sampling, which yields a more representative distribution of simulated attribute values with fewer realizations [2]. Here, term representative implies realizations spanning efficiently the range of possible conductivity values corresponding to the lognormal random field.

In this work we investigate the efficiency of alternative methods to classical LH sampling within the context of simulation of flow and transport in a heterogeneous porous medium. More precisely, we consider the stratified likelihood (SL) sampling method of [3], in which attribute realizations are generated using the polar simulation method by exploring the geometrical properties of the multivariate Gaussian distribution function. In addition, we propose a more efficient version of the above method, here termed minimum energy (ME) sampling, whereby a set of N representative conductivity realizations at M locations is constructed by: (i) generating a representative set of N points distributed on the surface of a M-dimensional, unit radius hyper-sphere, (ii) relocating the N points on a representative set of N hyper-spheres of different radii, and (iii) transforming the coordinates of those points to lie on N different hyper-ellipsoids spanning the multivariate Gaussian distribution. The above method is applied in a dimensionality reduction context by defining flow-controlling points over which representative sampling of hydraulic conductivity is performed, thus also accounting for the sensitivity of the flow and transport model to the input hydraulic conductivity field. The performance of the various stratified sampling methods, LH, SL, and ME, is compared to that of SR sampling in terms of reproduction of ensemble statistics of hydraulic conductivity and solute concentration for different sample sizes N (numbers of realizations). The results indicate that ME sampling constitutes an equally if not more efficient simulation method than LH and SL sampling, as it can reproduce to a similar extent statistics of the conductivity and concentration fields, yet with smaller sampling variability than SR sampling.

## References

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