Geophysical Research Abstracts
Vol. 21, EGU2019-3215, 2019
EGU General Assembly 2019

High-end solution techniques and accurate reference solutions: towards a community-wide benchmarking effort for stochastic inverse modeling of groundwater flow

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Geostatistical inversion refers to the problem of evaluating optimal estimates of spatial distributions for (typically hydraulic) properties, often associated with quantified uncertainty. To allow for a truly objective intercomparison and testing of new and existing methods, we pursue a benchmarking initiative for geostatistical inversion.

This initiative is grounded on the definition of a set of benchmarking scenarios. The first set is devoted to addressing fully saturated groundwater flow in multi-Gaussian and non-multi-Gaussian random fields of log-hydraulic conductivity. The key point of this initiative is that benchmarking efforts are much more powerful when individual methods are not just compared among each other but rather against highly accurate reference solutions for the ensuing best estimates, estimation variance,s and involved (multivariate) probability distributions.

Our study provides reference solutions and illustrates the high-end techniques we advance and develop to compute these solutions on massive high-performance computing equipment. We rely on Monte-Carlo Markov-Chain algorithms with a modified Metropolis-Hastings sampler, following the idea of preconditioned Crank-Nicholson (pCN) MCMC. This technique prevents the geostatistical prior from appearing in the rejection probability of MCMC, allowing geostatistical inversion at arbitrarily high spatial resolution. We combine the pCN-MCMC with a multi-tempered multi-chain approach, where diverse chains run at differing temperatures. The “hotter” chains enhance exploration of the solution space (tackling multi-modal solutions that can occur in non-linear inversion), the colder chains being devoted to performing the actual sampling.

We run these algorithms on the benchmarking scenarios and test their results thoroughly to enhance credibility to serve as reference solutions against which the quality of inversion methods can be appraised. The overall approach is free of any critical assumptions, the only approximation being the number of produced realizations (in the order of several hundred of thousands). While the invested computing costs may be extreme, we propose our accurate reference solutions to further assist and promote enhancing the community-wide research on increasingly efficient approximate inversion methods.