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

Wolfgang Nowak[1], Teng Xu[1], Sebastian Reuschen[1], Harrie-Jan Hendricks Franssen[2], and Alberto Guadagnini[3]
[1]Universität Stuttgart, Institute for Modelling Hydraulic and Environmental Systems (IWS), LS3 / Stochastic Simulation and Safety Research for Hydrosystems, Stuttgart, Germany (wolfgang.nowak@iws.uni-stuttgart.de)
[2]Institute of Bio- and Geosciences (IBG-3): Agrosphere, Forschungszentrum Jülich GmbH, Leo-Brandt-Strasse, 52425 Jülich, Germany
[3]Dipartimento di Ingegneria Civile Ambientale, Politecnico di Milano, Piazza L. Da Vinci 32, 20133 Milano, Italy

Geostatistical inversion modeling methods aim at characterizing spatial distributions of (typically hydraulic) heterogeneous properties from indirect information (e.g., piezometric heads, concentrations), while quantifying their uncertainties. Many methods have been developed, but only a few large intercomparison studies have been performed in the past decades. We present a benchmarking initiative for geostatistical inversion with the goal to enable a truly objective and accurate intercomparison and testing of new and existing methods.

This initiative defines an agreed-upon set of benchmarking scenarios. The benchmarking set focuses on addressing fully-saturated groundwater flow in multi-Gaussian log-hydraulic conductivity fields. Our study provides reference solutions and illustrates the high-end algorithms 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 MCMC (pCN-MCMC). In this technique, the acceptance probability of MCMC only depends on likelihood ratios, while being independent from the geostatistical prior. This largely improves acceptance rates and so reduces computational costs.

To further improve the accuracy and efficiency for Bayesian inversion of multi-Gaussian log-hydraulic conductivity fields, we combine pCN-MCMC with parallel tempering. Parallel tempering can handle the challenges associated with the need to explore large parameter spaces with possibly multi-modal distributions: it improves the efficiency of exploring the target posterior by exchange swaps between cold chains and hot chains that run in parallel, where the hot chains mainly explore the parameter space and colder chains exploit the identified high-likelihood regions.

Our new algorithm, hereafter termed pCN-PT, is tested against (a) accurate analytical solutions (kriging) in a high-dimensional, linear setting; (b) rejection sampling in a high-dimensional, non-

linear problem with only few measurements; and (c) pCN-MCMC in multiple independent runs in a high dimensional, non-linear scenario with sufficient measurements. These tests are also performed in the established benchmarking scenarios. We invite all interested researchers to test and compare different inverse modeling method(s) in these benchmarking scenarios.