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Efficient Geostatistical Inversion under Transient Flow Conditions in Heterogeneous Porous Media

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The assessment of hydraulic aquifer parameters is important for the evaluation of anthropogenic impacts on groundwater resources. The distribution of these parameters determines flow paths and solute travel times and is therefore critical for the successful design and deployment of remediation schemes at contaminated sites. Direct measurement of these properties is not possible, making indirect observations through dependent quantities and parameter estimation a necessity.

The geostatistical approach characterizes these hydraulic parameters without predetermined zonation. The parameter fields are treated as stochastic processes, optionally incorporating a priori information in the probability distribution. Maximizing the likelihood of the parameters with regard to the given observations yields a parameter estimate with high spatial resolution.

This approach naturally leads to nonlinear least squares optimization problems, namely objective functions of the form

$$L(Y) = \frac{1}{2}(Y')^T Q_{YY}^{-1} Y' + \frac{1}{2}\left[F(Y) - z\right]^T Q_{zz}^{-1}\left[F(Y) - z\right],$$

where Y are the parameters, Y' their deviations from the a priori estimate, Q_{YY} their covariance matrix, z the measurements, Q_{zz} their covariance matrix and F the forward model mapping parameters to observations. In theory, this objective function may be minimized using standard gradient-based techniques like Gauss-Newton. Due to the typically high number of parameters, however, this is not practical. Let n_Y be the number of parameters and n_z the number of observations. Then Q_{YY} and its inverse are both dense $n_Y \times n_Y$ matrices, and the sensitivity matrix $H_z := \partial z/\partial Y$ is a $n_z \times n_Y$ matrix that has to be assembled using forward or adjoint model runs.

Specialized schemes have been developed to reduce the dimensionality of the problem and avoid the high cost of handling products with Q_{YY}^{-1}. This enables efficient inversion in the case of a moderate number of observations as encountered in stationary inversion, where the cost of assembling H_z is in a reasonable range. Transient inversion, however, requires time series of measurements and therefore typically leads to a large number of observations, and under these circumstances the existing methods become unfeasible.

We present an extension of the existing inversion methods to instationary flow regimes. Our approach uses a Conjugate Gradients scheme preconditioned with the prior covariance matrix Q_{YY} to avoid both multiplications with Q_{YY}^{-1} and the explicit assembly of H_z. Instead, one combined adjoint model run is used for all observations at once. As the computing time of our approach is largely independent of the number of measurements used for inversion, the presented method can be applied to large data sets. This facilitates the treatment of applications with variable boundary conditions (nearby rivers, precipitation).

We integrate the geostatistical inversion method into the software framework DUNE, enabling the use of high-performance-computing techniques and full parallelization. Feasibility of our approach is demonstrated through the joint inversion of several synthetic data sets in two and three dimensions, e.g. estimation of hydraulic conductivity using hydraulic head values and tracer concentrations, and scalability of the new method is analyzed. A comparison of the new method with existing geostatistical inversion approaches highlights its advantages and drawbacks and demonstrates scenarios in which our scheme can be beneficial.