LA-UR- 04-1421

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Submitted to: The 15th International Conference on Computational Methods in Water Resources

Los Alamos
NATIONAL LABORATORY

A Markov Chain Monte Carlo Method for the Groundwater Inverse Problem

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In this study, we develop a Markov Chain Monte Carlo method (MCMC) to estimate the hydraulic conductivity field conditioned on the direct measurements of hydraulic conductivity and indirect measurements of dependent variables such as hydraulic head for saturated flow in randomly heterogeneous porous media. The log hydraulic conductivity field is represented (parameterized) by the combination of some basis kernels centered at fixed spatial locations. The prior distribution for the vector of coefficients θ are taken from a posterior distribution $\pi(\theta|d)$ that is proportional to the product of the likelihood function of measurements d given parameter vector θ and the prior distribution of θ. Starting from any initial setting, a partial realization of a Markov chain is generated by updating only one component of θ at a time according to Metropolis rules. This ensures that output from this chain has $\pi(\theta|d)$ as its stationary distribution. The posterior mean of the parameter θ (and thus the mean log hydraulic conductivity conditional to measurements on hydraulic conductivity, and hydraulic head) can be estimated from the Markov chain realizations (ignoring some early realizations). The uncertainty associated with the mean filed can also be assessed from these realizations. In addition, the MCMC approach provides an alternative for estimating conditional predictions of hydraulic head and concentration and their associated uncertainties. Numerical examples for flow in a hypothetic random porous medium show that estimated log hydraulic conductivity field from the MCMC approach is closer to the original hypothetical random field than those obtained using kriging or cokriging methods.

1. INTRODUCTION

Aquifer characterization by inverse models has attracted extensive research in the last two decades [1–4]. These groundwater inverse models may be classified into two groups: deterministic and stochastic models. In deterministic models, the aquifer is divided into a number of zones (with known boundaries) and regression-type techniques are used to adjust hydraulic properties of zones such that the modeled dependent variables (i.e., head and/or tracer data or concentrations) fit the measured values.

In the stochastic framework, the geostatistical method has been extensively used for solving inverse problems [5–13]. In the cokriging method, the estimate of log hydraulic conductivity at any location is represented as a weighted linear combination of all measurements on log hydraulic conductivity and dependent variables(hydraulic head and/or concentration). The weights in this linear combination are solved from a set of so-called cokriging equations, and the coefficients in these cokriging equations are covariances and cross-covariances between the log hydraulic conductivity and dependent variables. The parameters that define the mean and the covariance structure of the log hydraulic conductivity can be evaluated using, for example, the maximum likelihood method [5], and the cross-covariance between log hydraulic conductivity and dependent variables can be derived by solving adjoint state equations [12] and assuming a linear relationship between perturbations of log hydraulic conductivity and these dependent variables. The cokriging method can be applied to transient flow, i.e, head measurements at different times [12,14]. Harvey and Gorelick [13] presented a method for mapping the hydraulic conductivity field conditional to local direct measurements, hydraulic heads, and solute arrival time. The covariance matrices of head and arrival time are derived from linear approximations of the groundwater flow and transport. Unlike the deterministic approach, the cokriging method gives not only a mean prediction of log hydraulic conductivity (which is best linear unbiased estimator), but also an estimate of uncertainty associated with the mean prediction. Note that linearization is employed in the cokriging method in deriving cross-covariance functions between the perturbation of predictive variables (head, concentration, or travel time) and log hydraulic conductivity, while the relationship between log hydraulic conductivity and these predictive variables are nonlinear. The dependent variables solved using the cokriged hydraulic conductivity field in general will not honor their corresponding measurements. Yeh and his coauthors [15–17] developed a cokriging-based linear successive iterative approach which allows one to sequentially update hydraulic properties such that the modeled head values are close to observed values with a prescribed error. Hughson and Gutjahr [14] investigated the effect of conditional transient groundwater simulations on time dependent head data by an iterative cokriging approach. Their major conclusion was that significantly more accuracy and detail is obtained in the estimation of Y field using head measurements at steady state and additional time-dependent head data add some improvement but the gains are less.

The self-calibrated approach [18] is another geostatistical methodology for stochastic inverse modeling of groundwater flow. The method consists of two steps, generating a realization conditioned only on hydraulic conductivity measurements and adding a perturbation to the realization such that it is also conditional to head observations. The latter was fulfilled by parameterizing the perturbation as a function of perturbations at a few selected master locations and minimizing a penalty function (an objective function) that reflects the difference between the simulated and measured heads. To ensure that the perturbated transmissivity field honors transmissivity measurements, the set of master points must include all transmissivity measurement locations. The perturbation of transmissivity is updated in an iterative manner.

Woodbury and Ulrych [19] proposed a Bayesian approach to estimate transmissivity field from hydraulic head and transmissivity measurements for steady state flow. The parameters that govern the transmissivity field as a stochastic process are estimated using a maximum entropy method.

In this study, using the Markov Chain Monte Carlo method (MCMC), we develop an inverse model that accounts for both direct measurements of the log hydraulic conductivity and (steady state or transient) head measurements. The model has been tested for a two-dimensional saturated flow in a heterogeneous porous medium with variance $\sigma_y^2 = 2.0$.

2. STATEMENT OF THE PROBLEM

We consider transient water flow in saturated heterogeneous porous media satisfying the following continuity equation and Darcy's law:

$$S_s \frac{\partial h(\mathbf{x},t)}{\partial t} + \nabla \cdot \mathbf{q}(\mathbf{x},t) = g(\mathbf{x},t), \tag{1}$$

$$\mathbf{q}(\mathbf{x},t) = -K_s(\mathbf{x}) \nabla h(\mathbf{x},t), \tag{2}$$

subject to appropriate initial and boundary conditions. Here S_s is the specific storage, $h(\mathbf{x},t)$ is hydraulic head, $\mathbf{q}$ is the specific discharge (flux), $g(\mathbf{x},t)$ is a source/sink term, and $K_s(\mathbf{x})$ is saturated hydraulic conductivity. In this study, we treat $Y(\mathbf{x}) = \ln[K_s(\mathbf{x})]$ as a random function with mean $\langle Y(\mathbf{x})\rangle$ and covariance function $C_Y(\mathbf{x},\mathbf{y})$. We assume that there are n_Y measurements on log hydraulic conductivity $Y(\mathbf{x}_i)$, $i = \overline{1, n_Y}$, and n_h observation locations on hydraulic head measured at k different times. Now the problem we are facing is, given measurements $\mathbf{Y}_0 = (Y(\mathbf{x}_1), \cdots, Y(\mathbf{x}_{n_Y}))^T$ and $\mathbf{h}_0 = (h^{(1)}(\mathbf{y}_1), \cdots, h^{(k)}(\mathbf{y}_{n_h}))^T$, how to obtain an estimate of the true hydraulic conductivity field such that it honors both direct and indirect measurements. In addition, we are also interested in estimating the uncertainty associated with the estimation.

3. REPRESENTATION OF LOG CONDUCTIVITY FIELD $Y(\mathbf{x})$

Because the number of parameters (the number of nodes in discretization of the flow domain) being estimated in general is much larger than the number of measurements, parameterization is employed here. The log hydraulic conductivity field $Y(\mathbf{x})$ is represented by m basis kernels centered at some fixed spatial locations χ_j, $j = \overline{1, m}$,

$$Y(\mathbf{x}) = \sum_{j=1}^{m} \theta_j \, b(\mathbf{x}, \chi_j). \tag{3}$$

Here the kernels can be chosen as, for example, an exponential function $b(\mathbf{x}, \chi) = \exp[\sum_{i=1}^{d} (x_i - \chi_i)^2 / \lambda_i^2)]$, where d is the dimension of the domain D, and λ_i is a parameter that controls the influence of the kernels in i^{th} dimension. For the fixed basis kernels and given λ_i, the estimation of the log hydraulic conductivity field $Y(\mathbf{x})$ is computed from vector $\theta = (\theta_1, \theta_2, \cdots, \theta_m)^T$.

4. BAYESIAN INFERENCE

The essence of the Bayesian approach is Bayes' Theorem, which can be understood as a mathematical description of the learning process. Bayesian statistical inference requires *a prior* probability distribution for the parameters $\theta = (\theta_1, \cdots, \theta_m)^T$, which embodies our judgment before seeing any data $d = (d_1, \cdots, d_n)^T$ of how plausible it is that the parameters could have values in the various regions of parameter space. The introduction of a prior is the crucial element that converts statistical inference into an application of probabilistic inference. When we combine a prior distribution $\pi(\theta)$ for the parameters with the conditional distribution for the observed data we get a joint distribution for all quantities related to the problem:

$$\pi(\theta, d) = \pi(\theta)\pi(d|\theta) = \pi(d)\pi(\theta|d). \tag{4}$$

From this one derives Bayes' rule for the posterior distribution of the parameters given observed data d:

$$\pi(\theta|d) \propto L(d/\theta)\pi(\theta), \tag{5}$$

where $L(d/\theta)$ is the likelihood function. For the problem described above, the likelihood function of observed data $\mathbf{Y_0}$ and $\mathbf{h_0}$ for the given parameters θ can be written as

$$\begin{aligned} L(\mathbf{Y}_0, \mathbf{h}_0|\theta) \propto \exp&\left\{-\frac{1}{2}(\mathbf{Y}_0 - \mathbf{Y}_1)^T \textstyle\sum_Y^{-1}(\mathbf{Y}_0 - \mathbf{Y}_1)\right\} \\ &\times \exp\left\{-\frac{1}{2}(\mathbf{h}_0 - \mathbf{h}_1)^T \textstyle\sum_h^{-1}(\mathbf{h}_0 - \mathbf{h}_1)\right\}, \end{aligned} \tag{6}$$

where $\mathbf{Y}_1$ is a vector of the estimated log hydraulic conductivity values at the measurement points of Y, using (3) for given θ, $\mathbf{h}_1$ is the solution of head at observation points of h, solved from flow equations (1)-(2) using the estimated Y field, $\sum_Y^{-1}$ is an $n_Y \times n_Y$ matrix determined by observation errors and representativeness of measurements, $\sum_h^{-1}$ is a $(k\, n_h) \times (k\, n_h)$ matrix accounting for observation errors and model discrepancies on head h.

For Bayesian approach, we need to specify a prior distribution for θ. One such example is

$$\pi(\theta|\lambda_\theta) \propto \lambda_\theta^{m/2} \exp\left\{-\frac{1}{2}\lambda_\theta \sum_{i\sim j}(\theta_i - \theta_j)^2\right\} \propto \lambda_\theta^{m/2} \exp\left\{-\frac{1}{2}\lambda_\theta \theta^T W \theta\right\}, \tag{7}$$

where λ_θ is a hyperparameter, and $i \sim j$ represents the set of pairwise adjacencies, matrix W is defined as

$$W_{ij} = \begin{cases} -1 & \text{if } i \text{ and } j \text{ are adjacent}, \\ n_i & \text{if } i = j, \\ 0 & \text{otherwise}, \end{cases} \tag{8}$$

and n_i is the number of neighbors to location i. The prior distribution for the hyperparameter λ_θ in (7) can be chosen as a Gamma distribution

$$\pi(\lambda_\theta) \propto \lambda_\theta^{a-1} e^{-b\lambda_\theta}. \tag{9}$$

Finally, the posterior distribution of parameters (θ, λ_θ) given observed data $(\mathbf{Y}_0, \mathbf{h}_0)$ can be written as

$$\pi(\theta, \lambda_\theta|\mathbf{Y}_0, \mathbf{h}_0) \propto L(\mathbf{Y}_0, \mathbf{h}_0|\theta) \times \pi(\theta|\lambda_\theta) \times \pi(\lambda_\theta), \tag{10}$$

on which estimation and inference are based. Note that we only need to know the posterior distribution up to a constant proportionality for the Markov chain Monte Carlo simulations discussed in the next section.

5. MARKOV CHAIN MONTE CARLO SIMULATIONS

Sampling methods based on Markov chains incorporate the required search aspect in a framework where it can be proved that the correct distribution is generated at least in the limit as the length of the chain grows. Writing $\theta^{(t)} = (\theta_1^{(t)}, \cdots, \theta_m^{(t)})^T$ for the set of variables at step t the chain is defined by giving an initial distribution for $\theta^{(0)}$ and the transition probabilities for $\theta^{(t)}$ given the value for $\theta^{(t-1)}$. These probabilities are chosen so that the distribution of $\theta^{(t)}$ converges to that for θ as t increases and so that the Markov chain can feasibly be simulated by sampling from the initial distribution and then in succession from the conditional transition distributions.

Typically the Markov chain explores the space in a "local fashion". In some methods, for example, $\theta^{(t)}$ differs from $\theta^{(t-1)}$ in only one component of the state, e.g., it may differ with respect to $\theta_i^{(t)}$ for some i but have $\theta_j^{(t)} = \theta_j^{(t-1)}$ for $j \neq i$. Other methods may change all components at once but usually by only a small amount. Locality is often crucial to the feasibility of these methods. In the Markov chain framework it is possible to guarantee that such step-by-step local methods eventually produce a sample of points from the globally correct distribution. The procedure implemented in this study can be summarized as follows

1. Initialize parameters at some values $(\theta, \lambda_\theta)^{(0)}$. Theoretically, vector θ can be initialized by any numbers. For example, one can initialize θ by drawing a set of random numbers. In this study, we choose θ such that the initial conductivity field computed from θ is close to the kriged (or cokriged) field, i.e., choosing θ satisfying $\mathbf{B}\,\theta = Y_{kriged}$, or $\theta = (B^T B)^{-1} B^T Y_{kriged}$, where $\mathbf{B}$ is a matrix whose components are defined by the kernel function b in (3).

2. Update each θ_i according to the Metropolis rules:

   - Draw a value θ_i^* from the uniform distribution $U[\theta_i - r, \theta_i + r]$, where r is a pre-determined small number. Let θ^* be a vector that differs from θ only in their i^{th} component, i.e., replacing θ_i in θ by θ_i^*.
   - Compute $\alpha = \pi(\theta^*, \lambda_\theta | \mathbf{Y}_0, \mathbf{h}_0)/\pi(\theta, \lambda_\theta | \mathbf{Y}_0, \mathbf{h}_0)$. Accept new value θ_i^* (or θ^*) with probability $\min(1, \alpha)$, else reject new value θ_i^* (i.e., keep θ_i unchanged). In other words, if the newly proposed value increases the posterior probability (i.e., $\alpha > 1$), the new value is accepted. Note that even if the proposed value reduces the posterior probability (i.e., $\alpha < 1$), the value could still be accepted with a probability of α.

3. Update λ_θ given θ according to the following posterior distribution of λ_θ, again using the Metropolis rules

   $$\pi(\lambda_\theta | \theta) \propto \pi(\theta | \lambda_\theta) \times \pi(\lambda_\theta) \sim \Gamma(a + m/2, b + \theta^T W \theta/2), \tag{11}$$

   where a and b are two prescribed constants.

4. Repeat 2 and 3 until the chain converges.

To reduce the possible effect of starting values, some early iterations (called burn-in period) are discarded.

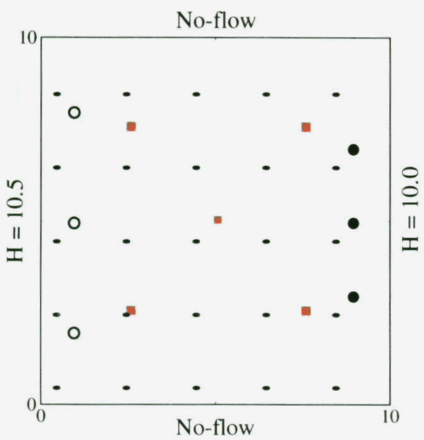

Figure 1. Layout of the problem configuration.

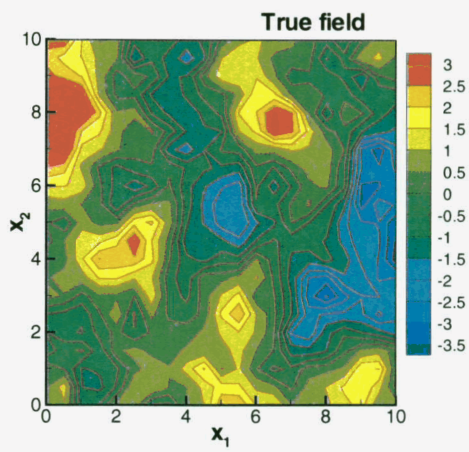

Figure 2. Reference log hydraulic conductivity field.

6. Numerical Examples

In this section we demonstrate the proposed inverse method for the case of two-dimensional flow in a saturated heterogeneous porous medium. The flow domain is a square of a size $L_1 = L_2 = 10$ (where the unit is any consistent length unit), uniformly discretized into 20×20 square elements. The no-flow conditions are prescribed at two lateral boundaries. The hydraulic head is prescribed at the left and right boundaries as 10.5 and 10.0 , respectively, which produces a mean flow from the left to the right. Three wells (solid cycles) located at $(9.0, 3.0)$, $(9, 5.0)$, and $(9.0, 7.0)$, as shown in Figure 1, pumping at deterministic rates of 0.3, 0.3 and 0.5, respectively.

We first generate a random field using specified mean and covariance function (mean log hydraulic conductivity $\langle Y \rangle = \langle \ln(K_s) \rangle = 0.0$, variance $\sigma_Y^2 = 2.0$, and an exponential covariance structure with a correlation length of $\lambda_Y = 2.0$) and consider it as the "true" field (reference field, Fig. 2) that will be estimated later using the proposed inverse method. We take $n_Y = 5$ samples from this field as direct measurements of log hydraulic conductivity (squares in Fig. 1). We then solve both steady state and transient flow equations using the true flow field to obtain both steady state and transient "true" head fields. For the steady state head field, we take head measurements at $n_h = 25$ locations (ellipses in Fig. 1), while for the transient flow we take head measurements at these 25 locations at different elapsed times.

After taking all these measurements, we pretend that the ensemble statistics (the mean, variance, and correlation length) used in generating the original Y field are not available any more and all we know are different kinds of measurements. Our purpose is to estimate the original hydraulic conductivity field using these measurements. As a first step, we may need to estimate sample statistics of the log hydraulic conductivity field. Several methods can be used to estimate the sample statistics (the mean, variance, and corre-

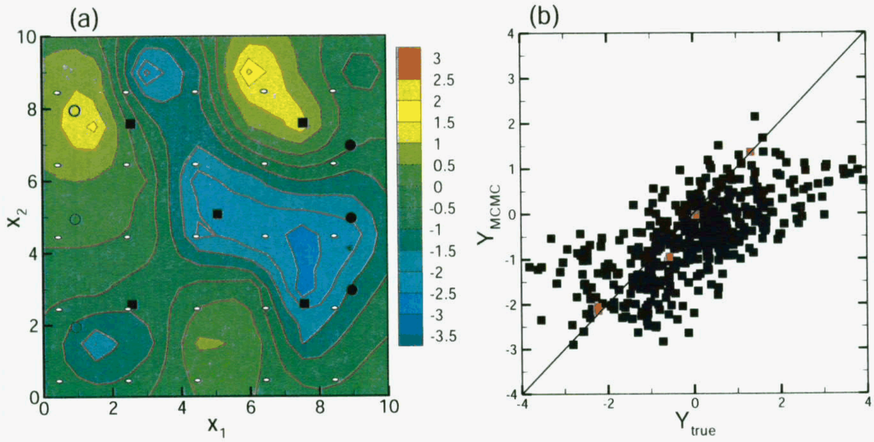

Figure 3. Inversion results from MCMC using both direct measurement and steady state head measurements, (a) Contour maps of the estimated log hydraulic conductivity field and (b) scatter plot showing comparison with ture field.

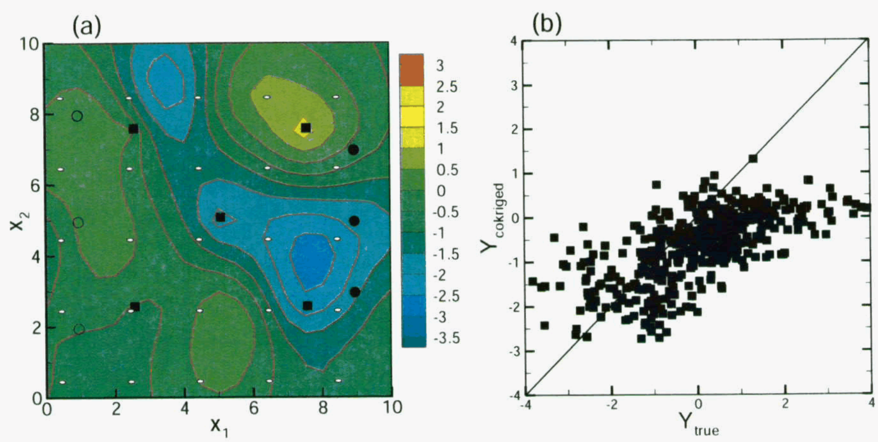

Figure 4. Inversion results from cokriging using both direct measurements and steady state head measurements, (a) Contour maps of the estimated log hydraulic conductivity field and (b) scatter plot showing comparison with ture field.

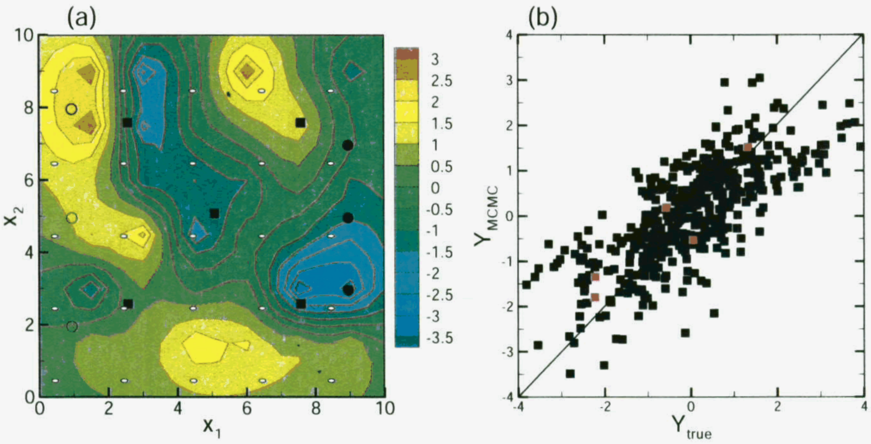

Figure 5. Inversion results from MCMC using direct measurements and transient head measurements at three times, (a) Contour maps of the estimated log hydraulic conductivity field and (b) scatter plot showing comparison with ture field.

lation length) of the log hydraulic conductivity. The simpliest way is to compute the mean and the variance from direct measurements and find the correlation length by variogram fitting. An alternative is to estimate these statistics from the maximum likelihood method using both direct and indirect measurements. In the Markov Chain Monte Carlo method (MCMC), these statistics can be estimated simultaneously in the inverse process. However, for simplicity and also for comparison with some other inverse methods (such as kriging or cokriging methods), in our preliminary study, we compute these statistics from direct measurements only. These estimates are $\langle Y \rangle = -0.739$, $\sigma_Y^2 = 2.33$, and a correlation length of $\lambda_Y \approx 1.5$.

For the MCMC method, based on the domain size and the estimated correlation length of about 1.5, we use a grid of 6×6 basic kernels locations, more-or-less uniformly distributed in the domain. The error matrices $\sum_Y$ and $\sum_h$ are chosen to be $\epsilon_Y I_{n_Y}$ and $\epsilon_h I_{n_h}$, where I_n stands for an identical matrix of $n \times n$ and ϵ's are prescribed standard deviations for errors of Y and h, respectively. Here we choose $\epsilon_Y = 0.03$ and $\epsilon_h = 0.003$. We tested the effect of the initial vector $u^{(0)}$ on the the final results by setting vector $u^{(0)}$ randomly or computing $u^{(0)}$ from the cokriged field and found that initializing $u^{(0)}$ using the cokriged field speeds up the convergence of the MCMC method, although two different initializations do not have significant impact on the final estimation.

We design several numerical examples. In the first example, we use the direct measurements and steady state head measurements only. The estimated log hydraulic conductivity field from the MCMC method is illustrated in Figure 3a in the form of a contour map. Figure 3b is a scatter plot showing comparison between the true field and the estimated field. Closeness of these two fields is measured in vision by how close the data points to the 45^o line. The red squares in the figure represent the values at 5 conditioning points. Comparing to the true field (Fig. 2), it is seen that the estimated field from the MCMC method not only captures the general structure of the original true field, but also contains some local details. Note that the estimated values at the conditioning points deviate from the values at the conditioning points in the true field, because the specified measurement errors in the MCMC method allow the estimated values vary within some ranges. The degree of such deviations is characterized by the standard deviation of errors specified by ϵ_Y.

For the purpose of comparison with the proposed method, we obtain an inverse solution using the cokriging method, where the unconditional mean and the unconditional exponential covariance structure (variance and correlation length) are taken from the sample statistics, the cross-covariance between head and log hydraulic conductivity is derived from first-order approximation of head perturbation, and the sensitivity of head perturbation to perturbation of log hydraulic conductivity is obtained from the adjoint method.

Figure 4 illustrates the estimated field from the cokriging method. It is seen that, while the inversed field from cokriging also captures the general structure of the original field (see Fig. 2), it lacks local details and is much smoother than both the original field and the field derived from the MCMC method. The reason is that, in cokriging, the relationship between the perturbation of head and that of log hydraulic conductivity is linealized while in fact it is not. The MCMC method adds some non-linearity that is ignored in the cokriging method.

In the second example, we use both direct measurements and transient head measurements taken at three elapsed times. We have tested the influence of different sets of elapsed times and found that measurements at early times have more important effect on inversion results. The reason is that, at the flow scenario as given in the example, the flow reaches the steady state condition very quickly, thus sets of head measurements taken at later times appear to be more correlated and information provided by these sets of measurements becomes less important. In this example, we take head measurements at t = 0.001, 0.1 and 1.0. The results are illustrated in Figure 5. The figure clearly shows that adding head measurements at early times has significantly improved inversion results.

7. Summary and Conclusions

In this study, using the Markov Chain Monte Carlo method (MCMC), we develop an inverse model that accounts for both direct measurements of the log hydraulic conductivity and (steady state or transient) head measurements. The model has been tested for a two-dimensional saturated flow in a heterogeneous porous medium with a unconditional variance $\sigma_y^2 = 2.0$. For an arbitrarily given statistics (the mean, variance, and correlation length) of log hydraulic conductivity, we generate a random field as the reference field, and then take both direct measurements from this field and (steady state and transient) head measurements solved from the reference field. The ensemble statistics (the mean, variance, and correlation length) of the field are estimated from these direct measurements and will be used in inverse modeling. It is demonstrated that the results from the MCMC method not only capture the structure of the reference field, but also reveal some local details. In addition, it seems that including transient head measurements makes significant improvements on inverse results.

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