Simulated-annealing-based conditional simulation for the local-scale characterization of heterogeneous aquifers

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Simulated-annealing-based conditional simulations provide a flexible means of quantitatively integrating diverse types of subsurface data. Although such techniques are being increasingly used in hydrocarbon reservoir characterization studies, their potential in environmental, engineering and hydrological investigations is still largely unexploited. Here, we introduce a novel simulated annealing (SA) algorithm geared towards the integration of high-resolution geophysical and hydrological data which, compared to more conventional approaches, provides significant advancements in the way that large-scale structural information in the geophysical data is accounted for. Model perturbations in the annealing procedure are made by drawing from a probability distribution for the target parameter conditioned to the geophysical data. This is the only place where geophysical information is utilized in our algorithm, which is in marked contrast to other approaches where model perturbations are made through the swapping of values in the simulation grid and agreement with soft data is enforced through a correlation coefficient constraint. Another major feature of our algorithm is the way in which available geostatistical information is utilized. Instead of constraining realizations to match a parametric target covariance model over a wide range of spatial lags, we constrain the realizations only at smaller lags where the available geophysical data cannot provide enough information. Thus we allow the larger-scale subsurface features resolved by the geophysical data to have much more due control on the output realizations. Further, since the only component of the SA objective function required in our approach is a covariance constraint at small lags, our method has improved convergence and computational efficiency over more traditional methods. Here, we present the results of applying our algorithm to the integration of porosity log and tomographic crosshole georadar data to generate stochastic realizations of the local-scale porosity structure. Our procedure is first tested on a synthetic data set, and then applied to data collected at the Boise Hydrogeophysical Research Site.

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1. Introduction

A key control on groundwater flow and contaminant transport in the subsurface is the spatial distribution of hydrological properties. Accurate characterization of these properties is crucial for developing reliable numerical models of flow and transport, which are required to design effective and cost-efficient aquifer remediation and groundwater management strategies. It is well understood that spatial variability needs to be defined at a wide range of scales for effective modeling of hydrological phenomena (e.g., Sudicky and Huyakorn, 1991; Gelhar, 1993; Zheng and Gorelick, 2003; Hubbard and Rubin, 2005). However, conventional hydrological measurement techniques tend to lie at two ends of a spectrum in terms of resolution and sampling volume, leaving a significant gap in a range that is expected to contain particularly critical hydrological information. Whereas pumping and tracer tests tend to yield only gross average properties over a relatively large region, core samples and borehole logs yield high-resolution estimates of aquifer properties, but only along sparse 1-D profiles. Consequently, over the past two decades, much work has been done on the use of geophysical methods for aquifer characterization. Such methods can bridge the gap between the analysis of cores or logs and well tests, and have proven to be extremely useful not only for aquifer zonation but also for estimating the spatial distribution of hydrological parameters (e.g., McKenna and Poeter, 1995; Hyndman et al., 2000; Chen et al., 2001; Troncic et al., 2002; Hubbard and Rubin, 2005; Kowalsky et al., 2005; Paasche et al., 2006). An important and still largely unresolved issue with the use of geophysical data in hydrological studies, however, is that of data integration. That is, how do we quantitatively integrate geophysical data with an existing database of other measurements to best constrain our knowledge of the spatial distribution of one or several target parameters?

The integration of different types of data for subsurface characterization has been a subject of much investigation in the petroleum industry, and has received increased attention in groundwater studies.
in recent years. Whereas much data integration and joint inversion work in the past has involved the determination of a single model of the subsurface parameters of interest, a number of recent efforts have focused on the creation of sets of multiple realizations that are consistent with all of the available data, and represent the uncertainty in our knowledge of the spatial distribution of subsurface properties (e.g., McKenna and Poeter, 1995; Bosch, 1999; Avseth et al., 2001; Caers et al., 2001; Mukerji et al., 2001; Ramirez et al., 2005; Hansen et al., 2006). The idea behind such conditional simulation approaches is that they can be used in combination with complex hydrological models to make predictions regarding groundwater flow and contaminant transport within a framework of uncertainty. Work with these methodologies has increased over recent years as a product of continually growing computer capacity, and also the ever increasing realization that “mean models” of subsurface properties do not adequately represent subsurface heterogeneity for reliable flow and transport predictions (e.g., Goovaerts, 1997).

Due to their inherent flexibility with regard to imposing constraints and their conceptual simplicity, simulated-annealing-type conditional stochastic simulations seem to be particularly promising for subsurface data integration (e.g., Deutsch and Wen, 1998, 2000; Kelkar and Perez, 2002). The simulated annealing (SA) approach is not limited to simple Gaussian statistics, and is able to incorporate any constraint on the output realizations that can be expressed in the form of an objective function, with the caveat that efficiency in terms of computation time and convergence decreases with constraint complexity. With SA, parameter fields satisfying all of the available data are obtained through minimization of a global, generally multi-component objective function, and multiple realizations can be generated by running the algorithm with different initial conditions. It should be emphasized that the variability seen in such multiple realizations depends on the applied constraints and stopping criteria, and as a result the realizations should not be confused with samples drawn from a posterior probability density function. Nevertheless, the SA method still allows evaluation of the variability in flow and transport behavior associated with uncertain data and constraints.

Recently, Tronicke and Holliger (2005) explored the use of SA for hydrogeophysical data integration through a synthetic model study. Starting with a simulated porosity model of a heterogeneous alluvial aquifer, they generated synthetic porosity logs and crosshole georadar traveltime data. These data, along with geostatistical constraints, were then used as conditioning information in a SA-based optimization procedure to generate porosity models that were consistent with all of the available information. In their work, Tronicke and Holliger (2005) pursued the classical SA approach of gradually “organizing” an uncorrelated random initial field through repeated swapping of values in the simulation grid, while adherence to the geophysical and geostatistical data was accomplished through matching the correlation coefficient between the realization and geophysical data to a prescribed value, and matching a prior parametric covariance model, respectively. Although the results obtained using this methodology clearly demonstrated that SA has much potential for hydrogeophysical data integration, we have found that the lateral continuity of the resulting porosity models is in general inadequate, which in turn significantly reduces the predictive value of such models in subsequent flow and transport simulations. Closer inspection indicates that this problem likely arises from the fact that it is inherently difficult with purely stochastic simulations to effectively impose constraints with regard to the underlying deterministic structure of the target parameter, as provided, for example, by high-resolution geophysical data.

In this paper, we present a novel SA-type conditional simulation procedure that aims to address and resolve this issue, as well as to improve the convergence and computational efficiency of the traditional SA method, which are known to be suboptimal as a result of having a relatively complex objective function. To begin, we review the overall methodology and describe an approach to more effectively account for the larger-scale deterministic information contained in geophysical data. Next, we test our conditional stochastic simulation algorithm on a synthetic data set consisting of crosshole georadar data and porosity logs from a highly heterogeneous, realistic aquifer model. Finally, we use our method to integrate field crosshole georadar and neutron porosity log data collected at the Boise Hydrogeophysical Research Site (BHRS) near Boise, Idaho, USA.

2. Conditional stochastic simulation using simulated annealing

2.1. Background

Simulated annealing is a directional Monte-Carlo-type optimization procedure, whose central idea is based upon the thermodynamics of a cooling melt. Atoms can move freely throughout a melt at high temperatures, but as the temperature is lowered, their mobility progressively decreases. Eventually, the system reaches its thermodynamic minimum-energy state and the atoms assume fixed positions within a crystal lattice. In SA, there are a large number of possible initial states, but during the cooling or annealing process all possible states converge to a final acceptable one. A flowchart describing the general methodology of SA for conditional simulation is shown in Fig. 1 (e.g., Deutsch, 2002; Kelkar and Perez, 2002; Tronicke and Holliger, 2005). The classical approach begins with an uncorrelated random field generated from an inferred/assumed probability distribution for the target parameter. The optimization process that follows consists of repeatedly perturbing individual values of this random field in order to satisfy a global objective function, $O$, which generally consists of the weighted sum of several component objective functions $O_i$ that represent constraints on fitting the output realization to the available data or information:

$$ O = \sum_{i=1}^{n} \omega_i O_i, $$

where $n$ is the number of component objective functions and $\omega_i$ are the weights. All perturbations that lower the global objective function are accepted in the algorithm, whereas those that do not are accepted according to a Boltzmann-type exponential probability distribution controlled by a temperature parameter $T$. This “decision rule” is
generally quantified in terms of the acceptance probability $p$ of a given configuration:

$$p = \begin{cases} 
1, & \text{if } O_{\text{new}} - O_{\text{old}} > 0 \\
\exp \left( \frac{O_{\text{old}} - O_{\text{new}}}{T} \right), & \text{otherwise.}
\end{cases} \quad (2)$$

The higher the temperature parameter $T$, the more likely an unfavorable perturbation will be accepted. Throughout the annealing process, the temperature is lowered gradually such that the model has a chance to reach an optimal energy state. Once the global objective function is deemed small enough, the SA process is terminated.

In the work of Tronicke and Holliger (2005) exploring the use of SA for hydrogeophysical data integration, the global objective function consisted of three components: the first controlled the reproduction of a specified covariance model for the porosity distribution to be simulated (inherently assuming stationarity and enforcing adherence to this model at a wide range of spatial lags), the second the reproduction of borehole porosity log data, and the third the conditioning of the simulated porosity field to the tomographic crosshole georadar image using a predefined target correlation coefficient between these quantities. Model perturbations during the SA procedure were made through the swapping of random values in the grid, which meant that the histogram of the original random realization did not change during the optimization procedure. Although, as mentioned previously, this work strongly demonstrated the potential of the SA method for generating aquifer models honoring a variety of data and prior information, it has become clear through further numerical studies that information with regard to the larger-scale subsurface structure, as provided by the geophysical data, is inadequately exploited, which in turn results in porosity models that are sub-optimal with regard to their internal structure and realism.

We believe that the above difficulty arises for a number of reasons. First is the issue of constraining the output porosity model to correspond to the geophysical image using only a single parameter, namely a prescribed correlation coefficient between these two quantities. In doing this, a rigid and arguably rather simplistic prior assumption is made about the relation between the geophysical data and the target parameter, which in many cases may be in error and cause difficulties with incorporating the geophysical information. One can imagine it being very difficult with a single parameter constraint to ensure that the accurate large-scale subsurface structural information provided by a geophysical image is properly retained in the output realizations. A second reason that we suspect contributes to the inadequate incorporation of large-scale geophysical information in the SA method of Tronicke and Holliger (2005) is the updating of the model through the swapping of values in the simulation grid. This implies the use of a pre-determined global probability density function for the target parameter, which is generally unknown and may be at odds with the information provided by the geophysics. Finally is the issue of constraining the experimental covariance of the output realizations to match a target covariance function over a wide range of lags. In doing this at large lags, adherence to larger-scale stochastic information is enforced, which in many cases may contradict the more accurate deterministic information contained in the geophysical image. In other words, because of our very limited knowledge of the true experimental covariance function at large lags, this constraint may force the output realizations to match an inaccurate covariance model, and thereby go against the large-scale information provided by the geophysical data.

### 2.2. Accounting for large-scale structural information

Given the above observations, our goal was to develop a new approach to SA-based conditional simulation that allows us to more suitably incorporate the larger-scale structural information contained in a geophysical image. The key concept in this approach is that high-resolution geophysical images, such as crosshole georadar or seismic tomograms, have as-of-yet largely unexploited potential in the conditioning of a model based on simulated annealing. In the following, we briefly outline our methodology.

#### 2.2.1. Perturb the model by drawing from a conditional distribution for the target parameter, given the available data

One key element of our new SA algorithm is the means by which we perturb the model and incorporate the geophysical and borehole log data into the output realizations. Instead of randomly swapping values in the simulation grid, we perturb the model by drawing from a conditional probability distribution for the target parameter, given these data (Deutsch and Wen, 1998). In other words, each perturbation step consists of drawing a random value from a conditional distribution, which can be defined for each cell of the model. This distribution is obtained given the available geophysical or log data and their relation to the target parameter, and provides the only means by which these data are incorporated into the simulation procedure. Around the boreholes the conditional distribution is obtained from the log data and their estimated uncertainty. Away from the boreholes, it is estimated from the geophysical data and their relation to the target parameter.

The above means of perturbing the model has several advantages in comparison to the traditional SA approach. In particular, it avoids the problem of requiring a priori the probability density function of the target parameter, and it offers significantly more flexibility in accounting for specific aspects and/or details of the geophysical information. For example, spatially dependent relationships consistent with varying degrees of local information can be readily incorporated into the simulation process without the need for objective functions to constrain the realizations to fit the different sources of information. The latter is of significant practical importance as it greatly contributes to the simplification of our global objective function, which in turn significantly improves the algorithm’s convergence and computational efficiency (Deutsch and Wen, 1998; Parks et al., 2000).

The question of how to best determine the conditional distribution for a particular target parameter with regard to geophysical data is currently receiving a significant amount of interest in a variety of domains (e.g., Ezzedine et al., 1999; Avseth et al., 2001; Chen et al., 2001; Bachrach, 2006). Although for hydrogeophysical applications the simplest approach is to attempt to relate the parameters using laboratory-derived petrophysical relationships, such relationships are usually only valid at the small scale, and tend to encounter problems when they are used to “convert” geophysical images to true subsurface properties. In an attempt to address this problem, Moysey et al. (2005) developed a Monte-Carlo approach involving numerical forward modeling to upscale petrophysical relationships from the laboratory scale to the scale of a geophysical survey. Day-Lewis et al. (2005) also addressed this issue by quantifying the correlation loss that occurs between a geophysical image and model of subsurface properties as a result of geophysical inversion. Another common method for estimating the conditional distribution for a hydrological parameter of interest given geophysical data, which we adopt in this paper because it is readily extended to field data and site-specific relationships, is to use collocated data sets along boreholes. Clearly, in this case, the quality of the estimated conditional relationship is dependent upon the number and quality of collocated data (e.g., Ezzedine et al., 1999; Chen et al., 2001; Bachrach, 2006; Paasche et al., 2006).

#### 2.2.2. Constrain realizations to parametric covariance model only at lags where the geophysical data do not provide enough information

The second key feature of our SA-type conditional simulation algorithm is the way in which we account for available geostatistical constraints. Instead of using the common approach of forcing the output realizations to match a target parametric covariance model over a wide range of spatial lags, we consider only those shorter lags...
where this information is required because it is not provided by the geophysical data.

It is well known that tomographic geophysical images can be viewed as smoothed versions of the corresponding true geophysical parameter fields. While being adequate representations of the underlying structure at larger-scales, such images lack information on the smaller-scale subsurface structure. This information can be adequately provided by geostatistical information regarding the parameter of interest. In our SA approach, we only constrain the output realizations to a parametric geostatistical model when necessary (i.e., at lags below the resolution threshold of the geophysical data), and we thus implicitly let the geophysical data have more control over the larger-scale structure of the output realizations. The choice of cut-off lag (i.e., the lag beyond which we do not constrain the output realizations to the target covariance model) must be chosen based on the estimated resolution of the geophysical image. That is, at scales where the subsurface structure is deemed to be not resolved by the geophysics, we should handle the variability statistically. Similar to our use of a conditional distribution for perturbing the model as described above, this approach towards geostatistical constraints contributes to the simplification of the global objective function of our SA procedure and thus to improved convergence and computational efficiency. In fact, the only objective function necessary in our algorithm involves constraining the output realization to the parametric covariance model at short lags. It should be noted that this procedure can be also viewed as effectively assigning a very high uncertainty to the target covariance function at large lags, thus allowing the geophysical data to control the large-scale structure in the output realizations. Clearly, using an approach that accounts for the ergodic variability in the covariance function (e.g., Ortiz and Deutsch, 2002; Hansen et al., 2008) in the SA objective function would accomplish a similar goal.

3. Application to synthetic data

We now apply our SA-type conditional simulation algorithm to a synthetic example. We use the same data that were used in Tronicke and Holliger (2005) such that the potential advantages and limitations of both approaches can be more easily identified. From an initial synthetic subsurface porosity model, crosshole georadar and neutron porosity log data were generated. The goal of the SA procedure was then to integrate these two data types and produce, within the bounds of uncertainty dictated by the limited information, realizations of the underlying porosity field. Crosshole georadar tomography has become a common tool for the detailed characterization of heterogeneous aquifers (e.g., Chen et al., 2001; Hubbard et al., 2001; Tronicke et al., 2002; Tronicke et al., 2004). Its strong potential for complementing and enhancing hydrological characterization comes from its high sensitivity to water content and the high spatial resolution of the method. We first describe below how the synthetic data were generated, and then the application of our algorithm for the data integration.

3.1. Porosity model

Tronicke and Holliger (2005) used a scale-invariant or “fractal” porosity model, 30 m long and 16.5 m deep, that was characterized by a von Kármán covariance function (von Kármán, 1948; Goff and Jordan, 1988):

$$C(h) = \frac{\sigma^2}{2^{1-\nu}} \Gamma(\nu) \left(\frac{h}{a_h}\right)^\nu K_\nu \left(\frac{h}{a_h}\right),$$

where $h$ is the lag vector, $a_h$ is the correlation length in the direction of the lag vector, $\sigma$ is the standard deviation, $\Gamma$ is the gamma function, and $K_\nu$ is the modified Bessel function of the second kind of order $0 \leq \nu \leq 1$, where $\nu$ is known as the Hurst number. The correlation length in Eq. (3) is related to the outer range of scale-invariance. Fig. 2a shows the synthetic porosity model that was generated from Eq. (3) using a spectral simulation technique. Best-fitting von Kármán parameters to the experimental variogram of this model are a $\nu$-value of 0.2 and correlation length of 2 m in the vertical direction, and a $\nu$-value of 0.3 and correlation length of 10 m in the horizontal direction. The realization has a mean porosity of 0.19 and standard deviation equal to 0.03. All of these parameters can be regarded as typical of unconsolidated clastic sediments consisting predominantly of sand and gravel (e.g., Gelhar, 1993; Heinz et al., 2003). The model is discretized at 7.5 cm increments and boreholes are considered at lateral positions of 0, 10, 20, and 30 m from the left model edge.

Key characteristics of the porosity model in Fig. 2a are that it is scale-invariant and thus characterized by strong heterogeneity at smaller scales and quasi-deterministic features, such as the central high-porosity channel, at larger scales. Having a $\nu$-value close to zero, the model emulates the seemingly ubiquitous “flicker noise” behavior characterizing virtually all petrophysical parameters including porosity (e.g., Walden and Hosken, 1985; Desbarats and Bachu, 1994; Hardy and Beier, 1994; Kelkar and Perez, 2002; Holliger and Goff, 2003) and can thus be regarded as a challenging, pertinent and realistic test case.

3.2. Database

From the porosity model in Fig. 2a, synthetic borehole porosity log data and crosshole georadar data were simulated. For the porosity log data, vertical traces from the model at the defined borehole locations were extracted. Consequently, the log data for this example are simply unbiased in-situ measurements of the actual porosity at the borehole locations with a resolution on the order of a grid cell (7.5 cm). Although this is clearly a simplification of real porosity log data, which will contain a small amount of smoothing related to the support volume of the measurement, we feel that it is an adequate approximation for the purpose of testing our approach.

To create the crosshole georadar data, three tomography surveys were simulated between all adjacent pairs of wells in the synthetic model (i.e., between 0 and 10 m, 10 and 20 m, and 20 and 30 m). Together, the data from these surveys allow us to reconstruct the subsurface velocity distribution in a series of panels having a width-to-depth ratio of approximately 0.66, which provides enough angular coverage of the inter-borehole region for high resolution tomographic velocity estimates (Williamson and Worthington, 1993). As a first
then tomographically inverted for the subsurface velocity distribution and travel times in a similar manner. The resulting traveltime data were used to see how the scale of heterogeneity in the synthetic model affected the picked velocities adjacent to the boreholes, plotted as a function of depth. Notice that, despite the fact that the tomographic velocities along the boreholes are clearly much smoother than the porosity logs for the reasons described above, we see a relatively strong negative correlation between the larger-scale, lower-frequency information in these data. That is, decreasing general trends in porosity are correlated with increasing general trends in tomographic velocity, and vice versa.

3.3. Conditional simulation

Using the synthetic data described above, the goal of our study was to generate plausible realizations of the subsurface porosity field. To do this using our algorithm, we first require a conditional probability distribution for porosity given the available data. To estimate this distribution for the georadar tomogram, we make use of the fact that we have collocated tomographic velocity and borehole porosity log measurements. As mentioned previously, this is a common approach for relating geophysical and hydrological parameters (e.g., Ezzedine et al., 1999; Chen et al., 2001) and is also quite realistic in near-surface aquifer characterization studies where crosshole tomographic data are often available.

Fig. 3 shows the porosity data at each borehole location (our synthetic porosity logs) and the crosshole georadar velocities adjacent to the boreholes, plotted as a function of depth. Notice that the data from all four boreholes have been pooled together. In both of the examples presented in this paper, we chose to estimate one conditional relationship from the velocity–porosity scatter plot that can be used throughout the entire modeling region. Clearly, this does not hold true for porosity, as different boreholes have different values and trends (as can be seen by the linear fit).

Fig. 4 shows a scatter plot of the velocity and porosity data from Fig. 3, where the data from all four boreholes have been pooled together. In both of the examples presented in this paper, we chose to estimate one conditional relationship from the velocity–porosity scatter plot that can be used throughout the entire modeling region. Clearly, this does not hold true for porosity, as different boreholes have different values and trends (as can be seen by the linear fit).

\[ \sqrt{\varepsilon_r} = \sqrt{\varepsilon_f} + (1 - \phi)\sqrt{\varepsilon_m}, \]

where \( \varepsilon_f = 80 \) are the relative dielectric permittivities of the dry matrix and water, respectively. For this study, a value of \( \varepsilon_m = 4.6 \) was employed, which is typical for unconsolidated sandy and gravelly sediments (e.g., Schön, 1998). For the electrical conductivity of the subsurface region, a constant value of 2 mS/m was assumed. Finally, because surficial soils and rocks are generally non-magnetic, it was assumed that the magnetic permeability is equal to its free-space value throughout the simulation region (e.g., Davis and Annan, 1989).

Using the above electrical properties, full-waveform georadar data were computed using a finite-difference time-domain (FDTD) solution of Maxwell’s equations in cylindrical coordinates (Holliger and Bergmann, 2002). This efficient and accurate computational method predicts all direct, refracted, reflected, and scattered electromagnetic waves and accounts for the inherent 3-D radiation and geometric spreading characteristics of dipole transmitters and receivers. The transmitter antenna was approximated as a vertical electric dipole emitting a Ricker wavelet with a center frequency of 100 MHz and a bandwidth of two to three octaves. Together with the uniform grid spacing of 7.5 cm, this wavelet yielded about 10 grid points per minimum wavelength, which was large enough to avoid numerical dispersion problems in the resulting data (Holliger and Bergmann, 2002). Corresponding dipole receiver antennas were emulated by recording the vertical component of the transmitted electric field. In each of the three crosshole data sets, 41 transmitter and 41 receiver locations were spaced equally at 0.375-m intervals between 0.75 and 15.75 m depth, yielding a total of 1681 traces per data set. After forward FDTD modeling, the traveltimes of the direct transmitted wavefield were determined using a commercial semi-automated picking procedure. No noise was added to the georadar data before picking in this example; however significant scattering due to the fine scale of heterogeneity in the synthetic model affected the picked travel times in a similar manner. The resulting traveltime data were then tomographically inverted for the subsurface velocity distribution using a nonlinear inversion scheme based on a finite-difference solution of the eikonal equation (Lanz et al., 1998). A combination of smallest and second-derivative-smoothness model regularization was employed in the inversion procedure, and the inversion cell length was 0.234 m.

Fig. 2b shows the image of electromagnetic wave velocity that was obtained from the tomographic traveltime inversion. A comparison of this image with the original porosity field in Fig. 2a demonstrates that the velocity tomogram outlines very well the larger scale subsurface structures such as the high-porosity channel in the center of the model. Conversely, structures smaller than the dominant georadar wavelength of approximately 1 m are not resolved in the tomographic image. The inherent smoothing of the image due to the band-limited nature of the radar signal, the applied regularization of the inverse problem, and the fact that only traveltimes were used for the reconstruction results in a loss of correlation with the original porosity model (Day-Lewis and Lane, 2004), and clearly demonstrates why we need additional information at smaller scales to generate realistic porosity realizations.

\[ \phi = \frac{\varepsilon_f}{\varepsilon_m} \]

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address the fact that the velocity–porosity relationship will in reality vary in space due to differences in tomographic resolution throughout the image plane (e.g., Day-Lewis and Lane, 2004; Moysey et al., 2005). However, it avoids significant complications and ambiguities associated with accurately estimating the spatially variable relationship, and it is a reasonable and pragmatic approach since the velocity resolution with crosshole georadar tomography is worst at the borehole locations. That is, in using the borehole-derived conditional relationship, we are using the most uncertain link between georadar velocity and porosity, which will mean greater variability in the resulting suite of realizations such that the simulations are under- rather than over-constrained by the tomography data.

To estimate the conditional distribution of porosity given georadar velocity from Fig. 4, we use a relatively simple parametric approach. Looking at the scatter plot, we assume a linear relationship with constant variance to be suitable. In other words, we assume that the conditional expectation of porosity \( \phi \) given the georadar velocity \( c \) takes the form

\[
E(\phi|c) = a \cdot c + b,
\]

and we solve for \( a \) and \( b \) by minimizing the mean squared error of the prediction. The variance \( \sigma^2(\phi|c) \) is then calculated using the following equation:

\[
\sigma^2(\phi|c) = \frac{\sum_{i=1}^{n} (\phi_i - E(\phi|c))^2}{n - np},
\]

where \( n \) is the number of values, \( \phi_i \) are the measured porosity values, and \( np = 2 \) is the number of parameters used in our linear model for the conditional expectation. Based on Fig. 4, we assume that the conditional distribution is approximately Gaussian, and thus that the
mean and variance are all the information that is required to draw values from the distribution. From the data we obtain $E(d_i) = -5.96e - 3 \times c + 0.71$ and $\sigma(d_i) = 0.017$. To generate the starting model and each perturbed value in the SA procedure, the above conditional distribution is used at every subsurface location except at the boreholes, where the distribution of porosity is more tightly constrained by the porosity log data. At the borehole locations, we chose to draw from a distribution having a conditional expectation equal to the log data and a small standard deviation of $\sigma = 0.005$.

What is left before running our SA algorithm is to define the geostatistical model for the porosity distribution, which is used to fill in the small-scale information missing in the tomographic data. For the vertical target covariance function, we use a von Kármán parametric model fitted to the porosity log data at short lags. This model is characterized by a correlation length of 2 m and a $r$-value of 0.2. We constrain the output realizations to this vertical parametric model for lags smaller than 2 m; that is, for spatial scales at which the geophysical data cannot provide reliable structural information. This cut-off value was chosen by comparing the vertical experimental covariances of the porosity log and tomographic data. Because the vertical parametric model can generally be considered as accurate, it was not varied in our simulations. The inherently limited knowledge of the horizontal covariance model, on the other hand, makes it necessary to run several realizations, varying this target function and trying to take into account its uncertainty. In the next section, we evaluate the effects of varying degrees of knowledge regarding the horizontal covariance structure. First, we use our best possible knowledge of the horizontal variability to consider the best result obtainable with our method. Then, we generate several realizations considering a more realistic, lower level of knowledge about the horizontal variability. In the latter case, the only information we have is that the correlation length from the velocity tomogram can be approximately considered as an indication of the maximum possible correlation length in the subsurface, and possibly some prior information regarding the aspect ratio between the vertical and horizontal correlation lengths. For all of the realizations in the next section, we fixed the limit of considered lags for fitting the horizontal target covariance function to 5 m. This cut-off value was chosen to be 2.5 times larger than the cut-off value used in the vertical direction because of the expected decreased resolution of the crosshole tomographic data in the horizontal direction as a result of survey geometry.

### 3.4. Results

In Fig. 5, we now show realizations obtained with different horizontal covariance constraints using our method, and compare them with the true porosity model (Fig. 5a). In addition, Fig. 5b shows the porosity model obtained by converting directly the tomographic image into porosity using the conditional expectation derived from the collocated data. As an initial test, we assumed extremely good knowledge of the horizontal target covariance function to evaluate the performance of our algorithm under the best possible scenario. Fig. 5c and d show two realizations obtained using the best fitting von Kármán parameters to the experimental horizontal covariance function of the true porosity model in Fig. 5a, but using different initial random realizations for the SA procedure. Notice that these realizations compare very favorably with the original porosity model in terms of small- and large-scale structures and the overall distribution of porosity values. The small-scale structures have been provided by the parametric target covariance function, the large ones by the tomographic georadar data, and the shape of the overall histogram by the borehole log data and our conditioning to the georadar velocities. We can therefore confidently say that, with proper integration of tomographic georadar data, borehole log data, and accurate knowledge of the small-scale vertical and horizontal variability, we have enough information to adequately simulate the detailed subsurface porosity distribution with our technique. It should be noted that small differences in the shape of the small-scale structures between Fig. 5c and d and the true model in Fig. 5a are the result of our using the best possible model fit to the true horizontal experimental covariance and not the experimental covariance itself. Also note that, not surprisingly, the quality of the tomographic image has an impact on the quality of the output realizations. For example, at the top and bottom of the modeling region, where a very low number of ray data exist due to the crosshole acquisition geometry, the simulation results in Fig. 5c and d are of limited reliability. Finally, concerning the small variability between Fig. 5c and d, the reason we do not see much difference between these realizations is because (i) the high-resolution radar tomographic data provide much information regarding the larger-scale subsurface structure, and (ii) the true subsurface model in this test case has a relatively long lateral correlation length, which means that the variability between the boreholes is limited.

In the next set of realizations shown in Fig. 5e–g we address the fact that, in reality, we have very limited knowledge of the horizontal variability of the target parameter. Here, we examine simulation results obtained using several different horizontal target covariance functions. To create Fig. 5e–g, we used horizontal correlation lengths of 10, 20, and 40 m respectively, which are 5, 10 and 20 times larger than the vertical correlation length of 2 m. Notice in these realizations that the lateral continuity increases with the horizontal correlation length, but only at scales smaller than the cut-off length because only the geophysical data are used to constrain the realizations at larger lags. In each case, the general distribution of porosity can be seen to be similar to that of the true porosity model. This is confirmed by Fig. 6, which compares the global porosity histogram of the true model with those obtained from the realizations. Although the observed variability in Fig. 5e–g is rather limited, we believe that this adequately represents our uncertainty about the subsurface structure when the geophysical information is taken into account. Also note that the realizations in Fig. 5e–g show a somewhat coarser aspect with respect to the smaller-scale structure when compared with the true model in Fig. 5a. This is a result of our limited knowledge of the horizontal correlation structure, and our thus using a $r$-value of 0.2, which was obtained from the borehole log data rather than the larger $r$-value characteristic of Fig. 5a, c, and d. This illustrates the importance of properly assessing the uncertainty in our underlying covariance model parameters, as our choice of these parameters clearly affects the results obtained. Finally, although we can consider the general aspect and connectivity of the subsurface porosity fields in Fig. 5e–g as very representative of the true porosity distribution, the hydrological accuracy of such conditional simulations can only be further evaluated through flow and transport simulations. Nonetheless, we can be confident that our approach shows significant improvement when compared to the more traditional SA approach (Tronicke and Holliger, 2005), for which one realization is shown in Fig. 5h.

![Histograms of the true porosity distribution shown in Fig. 2a (grey), the porosity log data (dotted) from Fig. 3, and the stochastic realizations of porosity in Fig. 5c–g (black).](image-url)
A last point of interest is the comparison of several experimental covariance functions for our synthetic example. In Fig. 7, the vertical and horizontal covariance functions of the true porosity model, borehole porosity logs, and georadar velocity tomogram are compared with those calculated from the realization in Fig. 5f. The experimental vertical covariance function of the realization clearly matches very well the target covariance function at small lags. Conversely, compared to the vertical covariance function of the tomographic data, the one corresponding to the realization shows major differences at small lags because the effects of smoothing have been replaced by small-scale structure based on the borehole porosity logs. In the horizontal direction, a major difference between the covariance function of the tomogram and that of the conditional stochastic simulation is visible at shorter lags due to tomographic smoothing, whereas at larger lags the overall character of the covariance functions is again rather similar. All of this helps to reinforce the fact that the experimental covariance function of the tomographic image cannot be used as a target covariance function. Instead, the tomographic image contains reliable deterministic structural information at larger lags that we incorporate into the realizations by drawing from a conditional distribution.

4. Application to field data

We now use our new SA approach to integrate crosshole georadar and porosity log data collected at BHRS near Boise, Idaho, USA, with the objective of simulating the detailed porosity distribution in this heterogeneous alluvial aquifer. The BHRS was established for the purpose of developing methodologies for joint geophysical/hydrological characterization of the 3-D distribution of hydrological parameters in unconsolidated heterogeneous alluvial deposits (Barrash and Knoll, 1998; Clement et al., 1999). The subsurface at the site is characterized by an approximately 20-m-thick alluvial layer consisting predominantly of gravel and sand with minimal fractions of silt and clay, which is underlain by a layer of red clay with a thickness of at least 3 m. At the time of the geophysical measurements (October 1998), the water table was at a depth of 2.96 m.

4.1. Database

The BHRS crosshole georadar data were acquired between two near-vertical boreholes (C5 and C6) which have a diameter of 10.2 cm and are approximately 8.5 m apart. The acquisition and processing steps used for the tomography are explained in detail in Tronicke et al. (2004). Here, we only summarize information relevant to the present study. The experimental setup consisted of 77 transmitter stations and 40 receiver stations spaced at 0.2 and 0.4 m intervals, respectively. All the transmitter and receiver positions were located within the saturated zone. Borehole deviations were measured using a magnetic deviation logging tool and were taken into account for the tomography. Due to the limited quality of the data, only 2064 traveltime picks from a total of 3080 georadar recordings were employed for the tomographic imaging. Preprocessing of the data included removal of the DC component and application of a 0–250 MHz zero-phase low-pass filter. The first-arrival traveltimes of the direct transmitted wavefield were determined using a commercial semi-automated picking procedure. The picked times were then tomographically inverted for the subsurface velocity structure using the same eikonal solver that was used in our synthetic example. Fig. 8 shows the resulting tomographic image. The velocity tomogram is distinguished by predominantly sub-horizontal structures, which is consistent with stratigraphic layering in the gravel and sand deposits at the BHRS (Barrash and Clemo, 2002). Also available were neutron
porosity log data, which were measured in boreholes C5 and C6 every 0.06 m (Barrash and Clemo, 2002).

4.2. Conditional simulation

As in the synthetic example, our first step towards integrating the available BHRS georadar and porosity log data was to estimate the conditional distribution of porosity given these data. Fig. 9 shows the porosity at each borehole location and the crosshole georadar velocity adjacent to the boreholes, plotted as a function of depth. As expected, the prominent variations in the porosity logs are also present in the tomograms along the boreholes, whereas the more subtle variations have generally no expression in the tomographic data. The average correlation coefficient between the georadar velocities and the neutron porosity logs is \( -0.51 \), whereas calculated independently along boreholes C5 and C6 the correlation coefficients are \( -0.61 \) and \( -0.36 \), respectively. Although the correlation between georadar velocity and porosity in borehole C6 is relatively low and will increase the uncertainty in the inferred conditional relationship between these parameters (compared to our synthetic example), these data still offer useful information. A possible explanation for the fact that the correlation along borehole C6 is worse than along borehole C5 could be that structural disturbances introduced during the drilling process are more severe for C6 than for C5. Such local disturbances in the immediate vicinity of the boreholes may have a significant influence on the porosity log data, but are unlikely to be reflected in the crosshole tomogram.

Fig. 10 shows a scatter plot of the velocity and porosity data from Fig. 9, where the data from both boreholes have been pooled together. Looking at this figure, we make again the assumption that the conditional expectation can be expressed as a linear relation. However, to capture the variability about the mean trend seen in Fig. 10, we assume that the conditional relationship between velocity and porosity is best described by a log-normal distribution. This decision was based on the analysis of porosity residuals about the best-fit line, as well as examination of the histogram of the porosity log data (Fig. 12), which shows a log-normal-type distribution instead of the normal-type distribution seen in Fig. 6. From the data we obtain \( E(\phi | c) = -9.41e^{-0.51c + 0.3} \) and \( \sigma(\phi | c) = 0.058 \) for the conditional expectation and standard deviation. To generate the starting model and for each perturbation in the SA procedure, values are drawn from this conditional log-normal distribution for every subsurface location except at the boreholes. Again, the distribution of porosity at the boreholes is more tightly constrained by the neutron porosity logs, and we thus draw from a conditional distribution with expectation given by the porosity values and standard deviation \( \sigma = 0.005 \).

Next, we must define a geostatistical model for the porosity distribution to fill in the small-scale information missing in the tomography data. For the vertical target covariance function, we again used a von Kármán parametric model fitted to the porosity log data at short lags. This model is characterized by a correlation length of 1.5 m and a \( \nu \)-value of 0.2, and was not varied in the simulations. Following the same reasoning as in our synthetic example, we constrained the realizations to this vertical parametric model at lags smaller than 2 m. For the horizontal target covariance function, we used a \( \nu \)-value of 0.2 and fixed the limit of considered lags to 5 m. Here, only the horizontal correlation length was varied in the simulations.

4.3. Results

Fig. 11 shows realizations obtained with our SA conditional simulation method using horizontal correlation lengths of 10, 15, 20 and 30 m, respectively, which are between 6 and 20 times larger than the vertical correlation length of 1.5 m. As in the synthetic case, notice that the lateral continuity increases with the horizontal correlation length, but only at scales below the cut-off length where the realizations were constrained to the covariance model. The general structure of the conditional simulations is also consistent with information regarding the true structure of the BHRS aquifer. In particular, we have the presence of three major geological units in depth having low, high, and medium porosity, respectively. In addition, all of the results show a striking degree of structural resemblance with a recently published time-domain full-waveform inversion of the crosshole radar data which has an expected resolution of less than half a meter in both the vertical and horizontal directions (Ernst et al., 2007). Based on this comparison, it appears that the models characterized by intermediate correlation lengths are likely to be more realistic than those characterized by the end-members of the considered range. Albeit circumspect, this evidence is consistent with information on the average ratio of the horizontal to vertical correlation length in alluvial aquifers compiled by Gelhar (1993). Moreover, it is important to note that the overall histograms of the modeled porosity structures are clearly of log-normal character and indeed compare very favorably with the histogram of the porosity logs (Fig. 12). The somewhat stronger presence of high porosity values in the stochastic realizations compared to the porosity logs could be the result of an incomplete representation of the borehole logs and/or a small overestimation of porosity due to the limited information available to constrain the conditional distribution inferred from the georadar tomography. On one hand, very high porosities of 50% have been reported at the BHRS (Barrash and Clemo, 2002). On the other hand, the available information limits the perfect characterization of the different units. It is conceivable that with more information regarding each of the three principal units and their distribution, more specific relationships could be used to characterize each unit separately, as for example the use of modal distribution or clustering methods (Hyndman et al., 1994; Troncic et al., 2004; Linde et al., 2006; Paasche et al., 2006) to define the conditional distribution of porosity given georadar velocity.

5. Conclusions

The main objective of this study was to develop a conditional stochastic simulation method that allows for the effective, quantitative integration of high-resolution geophysical data. We have developed a novel SA-based approach that demonstrates strong potential for generating highly detailed and realistic aquifer models honoring different data and prior information. A major advantage of our approach compared with related previous efforts is that deterministic information with regard to the larger-scale subsurface structure, as provided, for example, by tomographic geophysical images, is more thoroughly and appropriately incorporated into the resulting realizations. An additional advantage of this approach is that, because of a dramatically simplified global objective function, our algorithm exhibits very favorable
characteristics with regard to convergence and computational efficiency, and reduces the subjectivity associated with choosing the weighting of multiple objective function components.

Our new algorithm is defined by two key features. First, instead of swapping values within the SA simulation grid, we perturb the target field during the stochastic simulation procedure by drawing from a probability distribution for the output parameter, conditioned to the available data. For the synthetic and observed data sets considered in this study, we estimated the conditional distributions for the geophysical data using collocated georadar velocity and porosity measurements at the borehole locations, but clearly any appropriate alternative analysis technique could be used. Secondly, instead of constraining the stochastic simulations to match a parametric geostatistical model over a wide range of lags, we release this constraint at large lags and only enforce adherence to the covariance model at shorter lags that are not resolved by the geophysical data. In doing this, we let drawing from the conditional distribution correctly incorporate the larger-scale deterministic structure contained in the geophysical data.

Results of applying our new algorithm to both synthetic and field data sets were very positive. We found that the deterministic information with regard to the larger-scale subsurface structure, as provided by geophysical data, was properly incorporated into the output realizations, while the smaller-scale stochastic fluctuations were realistically represented by the parametric covariance models employed. Indeed, it can be argued that the resulting conditional stochastic simulations are characterized by an unprecedented degree of realism, which in turn is indicative of the fact that the proposed method capitalizes very well on the complementarity of the various data and constraints. Finally, it is important to note that the new conditional stochastic simulation approach presented here is quite generic and highly flexible and hence can be expected to be equally applicable to the quantitative integration of data from a wide range of geophysical, hydrological, and environmental techniques.

![Fig. 11. Stochastic realizations of the porosity distribution constrained by the BHRS georadar tomogram, porosity logs, and inferred vertical and horizontal target covariance models up to the cut-off lengths. The vertical target covariance model for all realizations was inferred from the available porosity logs and held constant ($\nu = 0.2$, $a_{\text{vert}} = 1.5$ m). The horizontal target covariance model was defined in (a)-(d) by $\nu = 0.2$ and $a_{\text{horiz}} = 10, 15, 20, 30$ m, respectively.](image)

![Fig. 12. Histograms of the porosity log data (dotted) and stochastic realizations of porosity in Fig. 11a-d (black).](image)
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