Stochastic modeling of complex nonstationary groundwater systems

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Abstract

Despite the intensive research over the past two decades in the field of stochastic subsurface hydrology, a substantial gap remains between theory and application. The most popular stochastic theories are still based on closed-form solutions that apply, strictly speaking, only for statistically uniform flows. In this paper, we present an efficient, nonstationary spectral approach for modeling complex stochastic flows in moderately heterogeneous media. Specifically, we reformulate the governing stochastic equations and introduce a new transfer function to characterize the propagation of system uncertainty. The new transfer function plays a similar role as the commonly used Green’s functions in classical stochastic perturbation methods but is more amenable to numerical solution. The compact transfer function can be used to construct efficiently various spatial statistics of interest, such as covariances, cross-covariances, variances, and mean closure fluxes. We demonstrate the advantages of the proposed approach by applying it to a number of nonstationary problems, including a large, complex problem that is difficult to solve by traditional methods. In particular, we focus in this paper on demonstrating the new approach’s ability to compute efficiently covariances and cross-covariances critical for measurement conditioning, monitoring network analyses, and stochastic transport modeling in the presence of complex mean flow nonstationarities (caused, e.g., by complex trends in aquifer properties, boundary conditions, and sources and sinks). This paper is an extension of our recent work that illustrated the basic approach for modeling nonlocal and nonstationary scale effects and uncertainty propagation in relatively simple situations.

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1. Introduction

Despite the intensive research over the past two decades in the field of stochastic subsurface hydrology, a substantial gap remains between theory and applications. The most popular stochastic theories are still based on closed-form solutions that apply, strictly speaking, only for statistically uniform flows [8,4]. Several researchers have recently been investigating general nonstationary flows in heterogeneous media in order to make stochastic modeling practical [30,16,17,39,13,20,18,5,44,45]. These researchers stressed that stochastic theories must be made much more flexible and efficient before they can be routinely applied to site-specific situations. In particular, Li et al. stressed [23,19] that many recently developed numerical perturbation techniques are very difficult to implement and, contrary to common expectation, may actually be more expensive than the classical Monte Carlo approach for problems of meaningful sizes. This is so because these techniques still require resolving small-scale heterogeneity and involve computing one or more huge “nasty” transfer function matrices relating the input and output fluctuations (e.g., the correlation functions, Green’s functions, or sensitivity derivatives). More quantitatively, Li et al. recently estimated that classical grid-based perturbation methods require $O(N^2)$ words of memory and between $O(N^2)$ and $O(N^3)$ floating point operations, where $N = O(L/k)^d$, $L$ being the characteristic problem size, $k$ the scale of heterogeneity, and $d$ the problem dimension.
This extreme degree of sensitivity of the computational cost to the problem size makes traditional stochastic perturbation techniques very difficult to implement for problems of realistic sizes and complexities.

In this paper, we present an efficient perturbation approach for modeling complex stochastic flows in moderately heterogeneous media. Specifically, we reformulate the governing stochastic equations and introduce a new transfer function to characterize the propagation of system uncertainty. The new transfer function plays a similar role as the Green’s function [30,39,13,14], sensitivity derivative [40,37,42,43,36,3], or covariance [38,7,15,26,27,11,44] in existing stochastic perturbation methods but is more amenable to numerical solution. The compact transfer function can be used to construct efficiently various spatial statistics of interest, such as covariances, cross-covariances, variances, and mean closure fluxes.

We demonstrate in this paper the computational advantages of the proposed approach by applying it to a number of nonstationary problems, including a large, complex problem that is difficult to solve by traditional methods. In particular, we focus in this paper on demonstrating the new approach’s ability to compute efficiently covariances and cross-covariances critical for measurement conditioning, monitoring network analyses, and stochastic transport modeling [11,12] in the presence of complex mean flow nonstationarities (caused by, e.g., complex trends in aquifer properties, boundary conditions, and sources and sinks). The paper is an extension of our recent work that illustrated the basic approach for modeling nonlocal scale effects [19] and uncertainty propagation [23] in relatively simple situations.

2. Problem formulation

To make our discussion more specific we consider steady-state flow in a saturated region where the hydraulic conductivity varies randomly over small spatial scales. The governing (head and Darcy) equations define implicit nonlinear relationships between the conductivity $K(x)$, hydraulic head $h(x)$, and the groundwater velocity vector $u_p(x)$

$$\frac{\partial}{\partial x_j} \left( K(x) \frac{\partial h(x)}{\partial x_j} \right) = 0 \quad x \in D \quad (1)$$

$$u_p(x) = -\frac{K(x)}{n} \frac{\partial h(x)}{\partial x_p} \quad (2)$$

with the boundary conditions

$$h(x) = h_b(x) \quad x \in \partial D_1$$

$$\nabla h(x) \cdot n(x) = 0 \quad x \in \partial D_2$$

Here and in subsequent equations we use indicial notation, with summation implied over repeated indices. In (1) and (2) the indices $j$ and $p$ range from 1 to the number of spatial dimensions $N_p$. For simplicity, we assume that the head equation applies over the $N_p$ dimensional spatial domain $D$ with perfectly known head $h_b(x)$ on the boundary $\partial D_1$ and no-flow conditions on $\partial D_2$ characterized by a unit normal vector $n$. These conditions determine the regional flow pattern. We suppose that the porosity $n$ is a perfectly known constant but the hydraulic conductivity, and therefore the head and groundwater velocity, are random functions of the spatial coordinate $x$.

For the particular problem considered here it is convenient to work with $f(x) = \ln [K(x)]$, the natural log of the hydraulic conductivity. In this case, (1) and (2) can be written:

$$\frac{\partial f(x)}{\partial x_j} \frac{\partial h(x)}{\partial x_j} + \frac{\partial^2 h(x)}{\partial x_j \partial x_j} = 0 \quad x \in D \quad (3)$$

$$u_p(x) = -\frac{\frac{\partial f(x)}{n} \frac{\partial h(x)}{\partial x_p}}{\partial x_p} \quad (4)$$

$h(x) = h_b(x) \quad x \in \partial D_1$  
$\nabla h(x) \cdot n(x) = 0 \quad x \in \partial D_2$

We wish to derive the ensemble covariances associated the conductivity, head, and velocity from these stochastic equations and from the joint probability density of the log conductivity at different locations. The joint density provides a complete statistical description of log conductivity variability.

3. The perturbation equations

Exactly deriving these covariances and other flow statistics from the log conductivity statistics, however, is generally impossible. Like most investigators [8,4,34], here we seek approximate results and work with linearized versions of the groundwater equations. In particular, we express the log conductivity, head, and velocity as random fluctuations around mean values:

$$f(x) = \bar{f}(x) + f'(x) \quad h(x) = \bar{h}(x) + h'(x)$$

$$u_p(x) = \bar{u}_p(x) + u'_p(x) \quad (5)$$

In each case, the mean value is indicated with an overbar and the fluctuation with a prime. When these expansions are substituted into (3) and products of fluctuations (second-order terms) are neglected the following approximate expressions for $\bar{h}$ and $\bar{h}'$ result:

$$\frac{\partial^2 \bar{h}}{\partial x_i \partial x_j} + \frac{\partial \bar{f}}{\partial x_i} \frac{\partial \bar{h}}{\partial x_j} = 0 \quad (6)$$
\[ \frac{\partial^2 h'}{\partial x_i \partial x_j} + \frac{\partial f'}{\partial x_j} = -\frac{\partial h}{\partial x_j} \frac{\partial f'}{\partial x_i} \quad (7) \]

\[ h'(x) = 0 \quad x \in \partial D_1 \]
\[ \nabla h'(x) \cdot n(x) = 0 \quad x \in \partial D_2 \]

The analogous expressions for \( \bar{u}_p \) and \( u'_p \) are obtained from (4)
\[ \bar{u}_p = -\frac{K_g}{n} \frac{\partial \bar{h}}{\partial x_p} \quad (8) \]
\[ u'_p = -\frac{K_g}{n} \left[ \frac{\partial \bar{h}}{\partial x_p} f' + \frac{\partial h'}{\partial x_p} \right] \quad (9) \]

where \( K_g = \exp(f'(x)) \) is the geometric mean of hydraulic conductivity.

The assumption that products of fluctuations can be neglected can only be justified when the fluctuation variances are relatively small [41,1,8]. Although more accurate higher-order approximations [22,24,45] can be introduced they do not change the basic points to be made here regarding computational effort. Note that the solutions to the first-order mean equations are identical to the deterministic head and velocity solutions obtained when \( f(x) \) is replaced by \( \bar{f}(x) \). The first-order perturbation equations provide useful additional information on deviations from these approximate means.

4. The nonstationary spectral method

Spectral methods offer a particularly convenient way to derive head and velocity statistics from linearized fluctuation equations such as (7) and (9). Utilizing these methods and invoking the assumption of statistical stationarity, Gelhar and his co-workers [2,8,9] developed a systematic framework for analyzing stochastic flows in heterogeneous media. But, of course, most hydrologic and hydrogeologic variables are not truly stationary. Papoulis [31] shows that the output (e.g., \( h', u' \)) of a linear transformations such as (7) and (9) is stationary only if the input (e.g., \( f' \)) is stationary and the transformations are spatially invariant. In the problem of interest here, spatial invariance implies that the fluctuation Eqs. (7) and (9) should have constant coefficients with the boundaries sufficiently distant having no effect on head and velocity fluctuations in the region of interest. Such spatial invariance requirement is clearly not met because, for most realistic groundwater problems, the coefficients \( \partial f'/\partial x_i \), \( \partial h/\partial x_i \), and \( \bar{u}_i \) may all vary significantly with \( x \) and possibly over time [11,25,35,20,30,16,44,45].

Li and McLaughlin [20,21] recently developed a generalized nonstationary spectral approach that does not require dependent fluctuations to be stationary. The stationary spectral representation is only applied to the original source of fluctuation \( f' \) (or the deviation from the \( \ln K \) trend):
\[ f'(x) = \int_{-\infty}^{\infty} e^{ikx} dZ_f(k); \quad (10) \]

and the dependent fluctuations are expanded in a generalized spectral representation characterized by a set of unknown complex-valued “ transfer functions” [20,32]
\[ h'(x) = \int \phi_{hf}(x,k) dZ_f(k) \quad (11) \]
\[ u'_p(x) = \int \phi_{u_p}(x,k) dZ_f(k) \quad (12) \]

The symbol \( k \) in (11) and (12) is the wavenumber (spatial frequency) and \( i = \sqrt{-1} \). The complex Fourier increment \( dZ_f(k) \), which is analogous to the random amplitude in a Fourier series expansion of \( f'(x) \), is defined implicitly by the relationship
\[ dZ_f(k) dZ_f(k') = S_{ff}(k) \delta(k' - k) dk dk' \quad (13) \]
where \( S_{ff}(k) \) is the spectral density of \( f'(x) \) and the superscript * indicates the complex conjugate. The Fourier increment can be viewed as a frequency domain representation of the random log conductivity fluctuation. If we take the expectation of the product \( f'(x) f'(x + \xi) \) and apply (10) and (13) we obtain the familiar relationship between the covariance and spectral density of \( f' \)
\[ P_{ff}(\xi) = \int_{-\infty}^{\infty} S_{ff}(k) e^{ik\xi} dk \quad (14) \]

The covariance and spectral density form a Fourier transform pair.

The transfer functions \( (\phi_{hf}, \phi_{u_p}) \) are introduced to account for possible nonstationary transformations because of the boundary conditions and variable mean gradients. An equation can be derived to determine each of the these transfer functions by substituting (11) and (12) into (7) and (9). The result is
\[ \frac{\partial^2 \phi_{hf}}{\partial x_i \partial x_j} + \frac{\partial f'}{\partial x_j} \frac{\partial \phi_{hf}}{\partial x_i} = -iK_g \frac{\partial h}{\partial x_j} e^{ikx} \quad (15) \]
\[ \phi_{u_p} = \frac{K_g}{n} \left( -\frac{\partial \bar{h}}{\partial x_i} e^{ikx} - \frac{\partial \phi_{hf}}{\partial x_i} \right) \quad (16) \]

\[ \phi_{hf}(x) = 0 \quad x \in \partial D_1 \]
\[ \nabla \phi_{hf}(x) \cdot n(x) = 0 \quad x \in \partial D_2 \]

Eqs. (15) and (16) are deterministic and complex-valued differential equations which have exactly the same structure and boundary and initial conditions as those of the original perturbation equations. If the linear transformations defined by (7) and (9) are strictly space invariant, the transfer functions obtained from (15) and
(16) will be the same as the harmonic transfer functions obtained from the stationary spectral theory. If, however, the transformations are spatially variant, the nonstationary transfer functions will not be the same as the stationary ones and will generally not be harmonic. The solutions to the transfer functions can be obtained by integrating (15) and (16) with respect to \( x \), with \( k \) treated as a parameter. The functions \( \phi_{hf} \) and \( \phi_{u_{ij}} \) obtained may be inserted into (11) and (12), which can then be used to derive the covariances and other flow statistics of interest in the same way as the classical stationary spectral method [8]

\[
P_{00f}(x, x') = \int_{-\infty}^{\infty} \phi_{00f}(x, k) \phi_{00f}(x', k) S_{ff}(k) dk
\]

where \( \theta \) represents any of the random processes \( f, h, u_1, u_2, u_3 \).

4.1. Computational issues and efficient solution techniques

To evaluate the covariances in (17), we need to find \( \phi_{hf} \) and \( \phi_{u_{ij}} \) from (15) and (16). In the special case of stationary flow, the transfer functions and related statistics can be obtained in a closed-form [8]. In certain special nonstationary situations with regular or infinite boundaries when the mean gradients are or can be expanded as the linear combinations of power, polynomial, harmonic, exponential functions and products of these elementary functions it may be possible to obtain analytical solutions or semi-analytical solutions to the transfer function equations.

In the most general case, however, the transfer functions and related covariance integrals must be evaluated numerically. This requires discretization of the transfer functions over space and frequency domains. Li and McLaughlin [20,18] discussed the computational advantage of the nonstationary spectral method, especially in terms of its memory efficiency, and presented a frequency dependent “multi-grid” solution technique that takes advantage of the different spatial scales of transfer functions at different frequencies. However, the nonstationary spectral method based on such a solution technique, though having removed the limiting memory problem associated with the moment methods, is still expensive. This is largely because of the fact that the transfer functions are oscillatory, and can be strongly oscillatory at high frequencies [due to the harmonic forcing, see Eq. (15)]. Covariance evaluations, however, require integrating the transfer functions over \( k_i \) from \( -\infty \) to \( \infty \), with fairly important contribution from high frequencies with a magnitude on the order of or greater than \( 1/\lambda \) (\( \lambda \) being the log conductivity correlation scale). Accurate solution of transfer functions at such high frequencies would require using a spatial grid spacing that is less than a fraction of the log-conductivity correlation scale. Such a grid limitation and the need to solve the transfer function equation repeatedly for different discrete frequencies make the nonstationary spectral method CPU intensive. Fundamentally, in terms of CPU, we still seem to be running into the often encountered phenomenon of “conservation of difficulty” as we go from one approach to another.

4.1.1. An efficient approach for solving the nonstationary transfer equations

In this section we present a new way for solving the nonstationary spectral equations. The new technique is based on the recognition that the forcing term in the head transfer function Eq. (15) is always of a separable form equal to a harmonic (oscillatory) function, \( \exp(ik_i x_i) \) (sources of numerical difficulty), times a coefficient related to the slowly varying mean gradient, \( \partial h/\partial x_i \) (source of analytical difficulty). This suggests that dependent transfer functions can also be expressed in a similar form,

\[
\phi_{hf}(x, k) = \psi_{hf} \exp(ik_i x_i),
\]

\[
\phi_{u_{ij}}(x, k) = \psi_{u_{ij}} \exp(ik_i x_i)
\]

where \( \psi_{hf} \) and \( \psi_{u_{ij}} \) represent the complex amplitude of the oscillatory head and velocity transfer functions. If we substitute (18) into (15) and (16), canceling out the harmonic functions on both sides and in the boundary conditions, the following equation can be obtained for determining each of the amplitude functions defined in (18),

\[
\frac{\partial^2 \psi_{hf}}{\partial x_j \partial x_i} + 2i k_i \frac{\partial \psi_{hf}}{\partial x_i} - k^2 \psi_{hf} + \mu_i \left( \frac{\partial \psi_{hf}}{\partial x_i} + i k_i \psi_{hf} \right) = i k_i J_i,
\]

\[
\mu_i \frac{K_n}{n} \left( J_i - \frac{\partial \psi_{hf}}{\partial x_i} - i k_i \psi_{hf} \right)
\]

\[
\psi_{hf}(x) = 0 \quad x \in \partial D_1
\]

\[
(\nabla \psi_{hf}(x) + i k \psi_{hf}(x)) \cdot n(x) = 0 \quad x \in \partial D_2
\]

where \( J_i \) is mean hydraulic gradient in \( x_i \) direction and \( \mu_i \) is mean slope in the log conductivity. Other notations were defined previously. It should be pointed out that the resulting amplitude Eqs. (19) and (20) as well as their boundary conditions involve no oscillatory forcing and are driven by the mean head gradient and the coefficients of these differential equations are smooth and depend only on the large-scale means or trends of the state variables involved. In the special case that flow transformations are strictly stationary, the amplitudes become spatially invariant. In general, the amplitudes are expected to vary smoothly over space and frequency. The following exact solution for two-dimensional flow in an infinite random conductivity field with a linear trend (15) clearly illustrates the behavior of the amplitude function \( \psi_{hf} \).
\[
\phi_{hf} \equiv \psi_{hf} \exp(ikx_i) = \left( \frac{-ik_i J_1}{k_1^2 + \mu^2 + 2ik_1} \right) \cdot \exp(ikx_i)
\]

where \(J_1 = -d\tilde{\theta}/dx_1\), and \(\mu = d\tilde{f}/dx_1\). There is no doubt that it would be dramatically easier to solve the equation that describes the smooth amplitude \(\psi_{hf}\) than that describing the original highly oscillatory transfer function \(\phi_{hf}\).

4.1.2. An efficient approach for nonstationary spectral inversion

To calculate the closure covariances and other statistics we still need to invert the transfer functions back to the space-time domain. The efficiency and robustness in numerical spectral inversion also affect the overall computational cost of the nonstationary spectral approach. Specifically, spectral discretization dictates for what and how many discrete wave numbers the amplitude equations [(19) and (20) where \(k_i\) is a parameter] have to be solved. If we substitute (18) into (17), the latter can be rewritten as

\[
P_{\theta_{hf}}(x, x') = \int_{-\infty}^{\infty} \psi_{\theta_{hf}}(x, k) \psi_{\theta_{hf}}^{*}(x', k) e^{ik(x-x')} S_{ff}(k) \, dk
\]

Numerical integration of (22) can be difficult since the kernel involved is generally oscillatory in the wave number domain and, at times, highly oscillatory when the spatial lag \(x_i - x'_i\) is large. If we are interested in calculating covariances and cross-covariances among different points [e.g., in application to sampling network design or measurement conditioning [18,12,42,43], use of a standard quadrature would require fine discretizations or measurement conditioning [18,12,42,43], use of a standard quadrature would require fine discretizations

\[
P_{\theta_{hf}}(x, x') = \int_{-\infty}^{\infty} \psi_{\theta_{hf}}(x, k) \psi_{\theta_{hf}}^{*}(x', k) e^{ik(x-x')} S_{ff}(k) \, dk
\]

Here we present a new way to evaluate the covariance integral. The new technique takes the advantage of the fact that the integrand in (22) is always of a separable form equal to a slowly varying function \(\psi_{\theta_{hf}}(x, k) \psi_{\theta_{hf}}^{*}(x', k) S_{ff}(k)\) (source of analytical difficulty) times an oscillatory harmonic function \(e^{ik(x-x')}\) (source of numerical difficulty) in the wave number domain. According to Davis and Rabinowitz [6], such a special separable type of oscillatory integrals can be efficiently and robustly evaluated from the following semi-analytical quadrature, by discretizing only the slowly varying amplitude functions:

\[
P_{\theta_{hf}}(x, x') = \sum_{e} \int_{e} \psi_{\theta_{hf}}(x, k) \psi_{\theta_{hf}}^{*}(x', k) e^{ik(x-x')} S_{ff}(k) \, dk
\]

where the integration is defined over a typical discrete rectilinear element in the frequency domain. The letter "\(e\)" represents a typical local element in which the slowly varying function \(\psi_{\theta_{hf}}(x, k) \psi_{\theta_{hf}}^{*}(x', k) S_{ff}(k)\) can be approximated as constant, linear, or other simple function of \(k\) so that the local element integration can be carried out analytically without discretizing the harmonic function. The summation is carried out over all discrete elements in the frequency domain. The resulting procedure is efficient since the number of \(k_m\) discretizations based on the slowly varying amplitude will be significantly smaller than it would otherwise be when the highly oscillatory harmonics have to be resolved.

In summary, we have presented a semi-analytic and semi-numerical solution technique both for transfer function solutions and covariance integrations. Taken together, we have at hand a highly efficient perturbation technique for solving distributed nonstationary stochastic groundwater problems. The new technique essentially takes care of the “numerically difficult” small-scale processes analytically and the “analytically-difficult” large-scale mean nonstationarity numerically. The efficiency of the new technique can be best appreciated if one considers a special stationary problem. In this case, the solution to the amplitude equation becomes numerically trivial, while numerical solutions using existing stochastic numerical methods, may well be computationally infeasible depending on the overall problem size relative to the scale of heterogeneity. Essentially, the new approach makes it possible to solve a nonstationary problem by only calculating numerically the “departure” from the stationary solution, or only the portion that makes the numerical solution necessary in the first place. Such innovations, having taken advantage of the nonstationary spectral representation, are perhaps not possible with other classical numerical methods formulated in the space-time domain. The new solution technique, together with the inherent parallel structure of nonstationary spectral formulation, and the extendibility of the nonstationary spectral method to general unsteady flow [20] will significantly increase the size and expand the range of site characterization problems that can be analyzed with stochastic methods.

5. Example and discussion

In this section we illustrate the distinct advantage of the reformulated nonstationary spectral method using three concrete examples of increasing degree of complexities. The objective is to demonstrate the viability of the proposed approach for practical stochastic groundwater modeling. Our first example illustrates the approach’s unique capability to model the correlation dynamics in heterogeneous media without having to resolve the small-scale heterogeneity. Our second example demonstrates that the innovation makes it possible to solve large stochastic flow problems that are difficult or impractical to solve using traditional methods.
Our third example shows the method’s ability to model large groundwater systems in the presence of complex sources/sinks, boundary conditions, and trends in aquifer properties.

**Example 1** (A simple flow situation). We begin by considering steady-state groundwater flow in the $x_1-x_2$ plane with deterministic no-flow conditions on the boundaries parallel to $x_1$ and constant head conditions on the boundaries parallel to $x_2$ (see Fig. 1). The log conductivity is an isotropic two-dimensional random field with a constant mean of zero, a variance of 1.0, and the following spectral density function [8,11,29]:

$$S_{ff} = \frac{2\sigma^2 \alpha^2 k^2}{\pi(k^2 + \alpha^2)^3}.$$  

(24)

The parameter $\alpha = 1.045/\lambda$. The correlation length $\lambda$ is 1.0 and the domain size $L$ is either 20$\lambda$ or 50$\lambda$. Other model inputs are shown in Table 1. The boundary conditions establish a uniform mean head gradient of 0.1 aligned in the $x_1$ direction. The resulting random head and velocity fields are most variable farthest from the boundaries.

This is a very simple stochastic flow problem with a nearly stationary solution that can be adequately approximated away from the boundaries by a closed form perturbation solution. For the inputs used here the closed form solution gives a head variance of 0.0046 [8] and velocity variances of 0.00375 and 0.00125 in the $x_1$ and $x_2$ directions, respectively [10].

We solve the problem by applying both the nonstationary spectral method and various traditional stochastic methods, including the Monte Carlo simulation (MC), moment method (MM), Green’s functions method (GM), adjoint state method (AM), and sensitivity derivative method (SM). We first consider a case in which all methods are applied over a relatively small domain of $L = 20\lambda$ with a fine spatial discretization of $\Delta x_1 = \Delta x_2 = \lambda/3$. This grid spacing allows resolving the small-scale heterogeneity and can be viewed as a benchmark which defines the correct solution. The number of Monte Carlo replicates is set equal to 20000 to minimize sampling errors based on a systematic probabilistic convergence analysis (see Fig. 2).

Fig. 3 shows the profiles in the $x_1$ direction of nine different combinations of covariances associated with the conductivity, head, and velocities. It is apparent that all methods compared give qualitatively similar results for this small problem. The linearized classical perturbation and nonstationary spectral methods compare well to the Monte Carlo method for this case.

Figs. 4–7 show results from a larger problem with $L = 50\lambda$ and coarser spatial discretizations. In this case the methods compared are no longer equivalent. As the grid spacing becomes larger than the correlation length both the classical perturbation and Monte Carlo methods (see Figs. 4–6) become inaccurate. This is especially the case for velocity related covariances which still do not appear to have converged when the grid spacing is reduced to $\Delta x = 0.5\lambda$. The computational requirements of the classical perturbation methods are excessive for values of $\Delta x$ smaller than 0.5$\lambda$ when $L = 50\lambda$. These results confirm that Monte Carlo and classical perturbation methods need to resolve small-scale heterogeneity at scales of $\mathcal{O}(\lambda)$ no matter how smooth the mean and variance distributions are. By contrast, the nonstationary spectral method (see Fig. 7) continues to give

| Table 1
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<td>Parameter definitions for Examples 1–3</td>
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<td>Domain length</td>
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<td>$\ln K$ variance (scale 1 and scale 2)</td>
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<td>$\ln K$ correlation scale (scale 1 and scale 2)</td>
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accurate solutions which are close to the approximate (linearized) infinite domain values of $\sigma_h^2 = 0.0046$, $\sigma_{hu}^2 = 0.00375$ and $\sigma_{uh}^2 = 0.00125$ cited earlier, even as the grid spacing used (to solve the transfer function equation) is increased to $20\lambda$.

Fig. 8 provides an informative graphical illustration of the reasons why the Monte Carlo and classical perturbation methods require fine discretization. This figure shows, for the example problem, spatial plots of the functions which determine the discretization requirements associated with each classical method. Fig. 8a (upper left) displays a set of typical Monte Carlo mean-removed head replicates (the mean head is a linear function of distance for this problem). If the groundwater flow solver used in the Monte Carlo simulation is to resolve the fine scale $[\xi(\lambda)]$ fluctuations shown in this figure its grid spacing needs to be smaller than $\lambda/2$. This

Fig. 2. Predicted head variance at the domain center by the Monte Carlo method as a function of the log conductivity variance for different number of realizations for Example 1.

Fig. 3. Comparison of the predicted covariances at the domain center as a function of the horizontal separation distance by the Monte Carlo method (MC), nonstationary spectral method (NSM), moment method (MM), adjoint state method (AM), Green’s function method (GM) using a high resolution grid for Example 1. The vertical separation distance is set equal to zero for autocovariances and to $\Delta x$ for cross-covariances.
requirement is generally recognized by investigators using Monte Carlo methods. It is less widely realized that similar requirements apply to classical perturbation methods. Fig. 8b (upper right) shows the cross-covariance $P_{fh}(x_1, n_1)$ that needs to be computed for the moment equation method. Each curve plots $P_{fh}(x, n)$ vs. $x_1$ for a different value of $n_1$. It is apparent that this cross-covariance, while smooth, changes significantly over scales of order $\lambda$, especially near the covariance function zero near $x_1 = n_1$. If these changes are to be resolved the moment equations must be discretized over a grid with a spacing no larger than $\lambda$, a value comparable to that required in the Monte Carlo approach.

Similar comments apply to the sensitivity derivative, Green’s function, and adjoint state methods. Fig. 8c (lower left) shows the Green’s/adjoint function $G(x_1, \zeta_1)$ that determines, together with the log conductivity covariance, the head and velocity variances in the Green’s function and adjoint state methods. Each curve plots $G(x_1, \zeta_1)$ as a function of $x_1$ for a different value of $\zeta_1$. Fig. 8d (lower right) shows the sensitivity derivatives for our example, also plotted as functions of $x_1$ for different values of $\zeta_1$. Both the Green’s functions and sensitivity derivatives change rapidly over scales of order $\lambda$, especially near the Green’s function peak at $x_1 = \zeta_1$. The only way to resolve these rapid fluctuations for all $\zeta_1$ is to use a uniform grid spacing smaller than $\lambda$. Here again, the discretization requirements are comparable to those encountered in Monte Carlo simulation.

The nonstationary spectral method is not limited by the factors illustrated in Fig. 9 because it does not require random fluctuations, covariances, Green’s functions, or sensitivity derivatives to be resolved. The hybrid space/wavenumber-dependent transfer functions which are the basis for the method usually vary over

Fig. 4. The effect of grid size on the accuracy of the predicted covariances at the domain center as a function of the horizontal separation distance by the moment equation method for Example 1. The vertical separation distance is set equal to zero for autocovariances and to $\Delta x$ for cross-covariances.
space in a way similar to the variance dynamics. In this example problem these functions are nearly constant over space except near the boundaries, where the increased curvature can be handled by adding a relatively small number of extra computational nodes. This is quite apparent from the transfer function $\psi_{2f}(x,k)$ plotted vs. $x_1$ in Fig. 9 (for the relatively high wave number $k_1 = k_2 = 0.5/\lambda$).

The nonstationary spectral method’s ability to account for small-scale variability with coarse spatial grids translates into a substantial computational advantage. It makes it possible to take advantage of the scale disparity between the variance dynamics and the small-scale heterogeneous processes. And when this scale disparity is large, as it is the case for most groundwater problems, the nonstationary spectral method will be significantly more efficient than classical stochastic methods.

**Example 2** (Flow in a large two-scale conductivity field). Our next example considers stochastic flow in a larger computational domain. The conductivity field is assumed to exhibit two disparate scales each characterized by the spectrum given in (24). The domain size is increased to 100 small-correlation scales (or 20 large-correlation scales). The boundary conditions are the same as those used in the previous example. Other model inputs are shown in Table 1.

Because of the increased domain size, stochastic modeling using classical methods becomes substantially more difficult. In fact, we are no longer able to solve the problem using the traditional perturbation methods on our 3GHz/2GB Pentium machine and it takes over two days to solve it using Monte Carlo simulation. Both the Monte Carlo and perturbation-based methods require using on the order of 100,000 nodes to resolve the small-scale processes and the resulting stochastic...
computations increase exponentially. In particular, the classical perturbation methods need to solve at least one to two hundred thousand, 100,000 by 100,000 matrix systems and store several 100,000 by 100,000 full correlation matrices. Although the Monte Carlo method is not limited by memory requirement on today’s computer, it still needs to perform on the order of 20,000 fine grid flow simulations in order to compute accurately the covariance statistics.

By contrast, the problem is easily solved using the nonstationary spectral method. In fact, it takes only 10 min on our computer to compute the spatial distribution of the head and velocity variances and all nine possible combinations of the covariances among the different flow variables (conductivity, head, and velocity) at a selected location. This high efficiency derives from the much smaller dimension of the new discretized transfer function and the fact that the spectral method only needs to resolve the variance distribution which is, in this case, virtually constant except near the boundaries. We adopt a grid spacing of $2\lambda$ for the transfer function solution in this example and evaluate the desired covariances from the transfer functions on a separate fine grid for plotting purpose.

Figs. 10 and 11 show the spatial distribution of a few selected covariances and cross-covariances obtained by the nonstationary spectral method and Monte Carlo simulation. Fig. 12 presents selected cross-covariance along a longitudinal profile. The covariances on the left two columns in Figs. 10 and 11 are obtained using the spectral method on two different grids of, respectively, $\Delta x = 2\lambda$ and $\Delta x = \lambda$. The covariances on the right column of these figures are obtained using the Monte Carlo simulation on a fine grid of $\lambda/3$. The fact that the coarse grid spectral solutions are virtually identical to the more expensive fine grid spectral solutions and reasonably close to the much more expensive Monte Carlo solutions demonstrates the efficiency, accuracy,
and potential of the proposed method for large-scale modeling.

It is interesting to note that the predicted covariances, especially the velocity covariances, show a “self-similar” two-scale structure in response to the two-scale conductivity field. The unique capability of the new method in allowing predicting the embedded fine-scale correlation dynamics using a grid that is much larger than the small correlation scale is extremely interesting. This capability is particularly significant for modeling multi-scale correlation dynamics and for solute transport modeling since both small and large scale velocity variabilities contribute importantly (but in a different way) to field-scale plume migration [28,33].

**Example 3** (Flow in the presence of more complex conductivity trends and sources/sinks). Our final example considers a complex flow situation that illustrates the approach’s ability to adapt to a realistic field environment. The problem involves different types of boundary conditions, distributed and localized sources and sinks, and a conductivity field that exhibits both a systematic variation and random heterogeneity around it. The domain size is the same as that used in the previous test case, equal to 100 small correlation scales. The spatial structure of the random fluctuations around the trend is also assumed to be the same as that in the previous example. The mean conductivity is assumed to be a smooth function generated from a realization of a random field with a variance of 0.5 and correlation scale comparable to (equal to one fifth of) the overall simulation domain. The aquifer is confined and bounded on the west and south side by no flow conditions and on the north and east by constant head conditions. Other inputs are shown in **Table 1**.

Again due to the large domain size, the computations utilizing classical stochastic perturbation methods are excessive. By contrast, the problem is solved
relatively easily using the nonstationary spectral method. In this case, we use a grid of \( \Delta x = 2\lambda \), a value selected conservatively to resolve the complex nonstationary mean distributions, and it takes approximately 10 min of CPU to solve the problem on our Pentium 4 desktop.

Fig. 13 shows the predicted nonstationary mean head and velocity distribution. The flow is derived from recharge and drained toward the well and two constant head boundaries to the north and east. Fig. 14 presents the spatial distribution of the head variance, which is, as expected, highly nonstationary because of the complex spatial distribution in the mean flow. The predicted variance is high where the head gradient is large, especially in the area around the pumping well. The head variance is zero at constant head boundaries. Fig. 15 shows a typical transect of the mean head distribution and the associated one standard deviation confidence interval. The solid line represents the fine grid (\( \Delta x = \lambda \)) solution, for verification purpose, and the unconnected open symbols the coarse grid solution (\( \Delta x = 2\lambda \)). The excellent match between the fine and coarse grid solutions confirms the accuracy of the latter and the efficiency of the nonstationary spectral method for modeling complex groundwater systems.

Figs. 16 and 17 show the spatial distribution of a few selected covariances at a representative location obtained by the nonstationary spectral method. Unlike in the earlier examples, the covariance distributions in this case are no longer symmetric and the correlation between the random variables of interest at two different points are strongly nonstationary and depends on their absolute locations. This strong nonstationarity was also noted in [46] and implies that the commonly used empirical approach to estimate the spatial covariance
structure directly from limited field data based on the stationarity assumption can be problematic and violates the underlying principle of conservation of mass. Again, the good agreement between the fine and coarse grid covariance solutions confirms the accuracy of the latter and the efficiency of the nonstationary spectral method.

6. Summary and conclusions

We have presented an efficient approach for modeling uncertainty and complex correlation dynamics for groundwater flows in moderately heterogeneous aquifers. The reformulated spectral technique provides a compact, low dimension transfer function and allows modeling multi-scale dynamics without having to solve numerically the fine scale dynamics and thus significantly increases the size and scope of the problems that can be solved by stochastic modeling. In particular, the nonstationary spectral approach makes it possible to evaluate groundwater model accuracy or quantify the uncertainty caused by unmodeled small-scale heterogeneity and provide physically-based covariances needed for stochastic inverse modeling, and stochastic transport modeling under more realistic conditions for problems of meaningful sizes.

We have emphasized computational issues in this paper because numerical limitations have greatly restricted the application of stochastic methods to real-world problems. At present the most useful stochastic tech-
Techniques are based on closed-form solutions which depend on stationary assumptions or other specialized requirements. In a sense, this situation is analogous to the state of deterministic groundwater modeling several decades ago, before efficient numerical methods became widely popularized.

Classical numerical methods for solving stochastic groundwater problems need to resolve variability over small spatial scales. Monte Carlo methods need to...
resolve the random fluctuations in each replicate simulated, moment equation methods need to resolve cross-covariance functions that vary rapidly when their two spatial arguments are close, and the Green’s function and sensitivity derivative methods need to resolve Green’s functions and sensitivity derivatives that both vary over relatively small scales. We have seen that all of these classical methods require computational grids with cell lengths approximately 1/3 of the log conductivity correlation length. This can lead to very large computational grids and high CPU and memory demands when the domain size is large compared to the correlation length.

The nonstationary spectral method offers a convenient and efficient alternative to computationally unwieldy Monte Carlo and perturbation methods. This method is effective because it combines the best features of analytical and numerical techniques. The statistically stationary small-scale portion of natural variability is described with a compact spectral (Fourier) representation while the remaining nonstationary component is described as a larger-scale spatial process driven by mean gradients. The numerical computations focus on departures from stationarity. The division of labor is not prescribed explicitly but is handled naturally with transfer functions that depend on both wavenumber and location. Discretized numerical computations are performed on spatial grids that are comparable in size to the grids used in traditional deterministic modeling applications. The result is a significant decrease in the computational effort needed

Fig. 13. Spatial distribution of mean head and velocity distribution for Example 3; The background image represents the mean lnK distribution.

Fig. 14. Spatial distribution of head variance obtained on a coarse grid ($\Delta x = 2\lambda$) by the nonstationary spectral method for Example 3.

Fig. 15. Comparison of the predicted head distribution with one-standard deviation confidence interval on a coarse grid ($\Delta x = 2\lambda$) and fine grid ($\Delta x = \lambda$) by the nonstationary spectral method for Example 3.
to compute statistics such as head and velocity covariances.

The nonstationary spectral method, like classical perturbation methods, relies on the small perturbation assumption. This may not be a major limitation in many groundwater flow applications, including the problem examined here. Large-scale changes in log conductivity that increase the variance around a constant mean can often be treated as nonstationarities (e.g., trends) since the method does not require that the log conductivity mean be constant. This has the effect of decreasing the variance of deviations from the mean, making the small perturbation assumption more defensible. The method can also handle a number of other generalizations not discussed here, including time dependence, random boundary conditions, and the use of higher-order perturbation approximations [20,21].

The method’s requirement that all uncertainty must ultimately be related to stationary random parameters may seem to be a significant limitation. In reality, this requirement reflects a very important tacit assumption of stochastic groundwater hydrology. To be specific, suppose we wish to know how predicted head or flux uncertainty is affected by spatial variations in hydraulic conductivity. A number of probabilistic methods, including the one described here may be used to infer the (possibly nonstationary) ensemble statistics of head and velocity from the ensemble statistics of hydraulic conductivity. In order to apply any stochastic methods to practical problems, we need to obtain estimates of the conductivity statistics which form the basis for our stochastic analysis. In practice, these statistics are typically derived from a limited number of field measurements. In most situations the only type of parameter nonstationarity that we can hope to infer from field data is a large-scale trend in the local mean. The nonstationary spectral method can accommodate such trends since it requires that the mean removed parameter be stationary. This suggests that the method’s requirement that uncertainty be related to stationary random parameters is really not a practical limitation. We need to do this any way if we want our analysis to rely on data gathered in the field.

In summary, the nonstationary spectral method makes it possible to model the uncertainty and correlation dynamics in statistically nonuniform flow, as a part of groundwater modeling. The effort required is greater than a traditional deterministic simulation but the increase depend much less on domain size than traditional methods and is moderate enough to be tolerable in many applications. In fact, this increase in computational effort is especially easy to accept since it offers
the opportunity to assess groundwater model uncertainty in a scientifically credible way.

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Fig. 17. Spatial distribution of predicted velocity covariances at a typical point obtained on coarse grid \((\Delta x = 2\lambda)\) by the nonstationary spectral method for Example 3.


