Prior mapping for nonlinear flows in random environments

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We analyze nonlinear flows in randomly heterogeneous environments, which are characterized by state-dependent diffusion coefficients with spatially correlated structures. The prior Kirchhoff mapping is used to describe such systems by linear stochastic partial differential equations with multiplicative noise. These are solved through moment equations which are closed, alternatively, either by perturbation expansions, or by a posterior linear mapping closure. The latter relies on the assumption that the state variable is a spatially distributed Gaussian field. We demonstrate that the former approach is more robust.

According to general diffusion theory, the flux of substance, $\mathbf{u}$, is down gradient of the system state, p, i.e., $\mathbf{u} = -K\boldsymbol{\nabla}p$. Quite often, the environment is heterogeneous and the coefficient of proportionality K depends on the system state, $K = K(\mathbf{x},p)$. In most applications, K cannot be known precisely in all of its relevant details. For example, predicting flow and transport in subsurface environments is complicated by the high degree of heterogeneity and the lack of detailed characterization of their hydraulic properties. By the same token, modeling semiconductor fabrication must take into account the presence of impurities whose location and density are seldom known *a priori*. Consequently K should be treated as a random variable, so that the corresponding equations become stochastic [1,2].

To be specific, we formulate the problem in terms relevant to gas flow through porous media. Then $\mathbf{u}$ and p denote the Darcian (macroscopic) flux and the gas pressure, respectively. Hydraulic conductivity of the medium, K, is related to its permeability k through $K = k/\mu(p)$, where μ is the gas viscosity. Assuming isothermal conditions with temperature T and constant chemical composition, density of a real gas can be expressed as $\rho(p) = p/[Z(p)RT]$, where $Z(p)$ is the compressibility factor and R is the gas constant. Then, in the steady-state regime, accounting for the conservation of mass yields the nonlinear flow equation,

$$\boldsymbol{\nabla}\cdot[D(\mathbf{x},p)\boldsymbol{\nabla}p]=0, \quad D(\mathbf{x},p)\equiv k(\mathbf{x})\frac{p}{\mu(p)Z(p)}. \quad (1)$$

If properties of a porous medium are highly varying and uncertain, k can be conveniently treated as a correlated random field [3].

Such stochastic partial differential equations (PDEs) are notoriously hard to analyze due to the nonlinearity of the spatially correlated multiplicative noise. Linear stochastic PDEs, such as Eq. (1) with $D=D(\mathbf{x})$, can be successfully analyzed through the moment equations [4,5]. This approach typically relies on perturbation expansions to close the system, but alternative methods, such as Gaussian approximation [6], are also available. However, direct application of the moment equations method to Eq. (1) would require either expanding $D(p)$ into Taylor series about (ensemble) mean pressure, $\langle p \rangle$, or a simple linearization $\langle D(p) \rangle \approx D(\langle p \rangle)$. Both approaches can hardly be considered satisfactory since their validity cannot be assessed *a priori*. For example, a similar linerization used in a study of the interface dynamics in random media was shown to be less than optimal [7].

On the other hand, stochastic PDEs with nonlinearities stemming from the presence of nonlinear source terms proved to be amenable to approaches which rely on deriving the probability density function (PDF) for the system state [8,9]. Mapping closures are usually used to derive the closed-form PDF equations [10,11]. While PDF approaches treat nonlinear source terms exactly, their applicability to systems with nonlinear multiplicative noise of the kind presented in Eq. (1) is less clear. Application of the linear Gaussian mapping to an equation similar to Eq. (1) proved to be successful only under limited conditions [12].

In this Rapid Communication, we employ the Kirchhoff mapping to the stochastic flow equation (1) prior to its ensemble averaging. Moment equations are then derived for the resulting linear PDE, and the closures are obtained by a perturbation expansion. We assess the quality of our predictions, and the validity of our perturbation expansion, by comparing them with Monte Carlo simulations (MCS) of Eq. (1). These consist of (i) generating multiple realizations of the permeability field $k(\mathbf{x})$ with a given correlation structure, (ii) solving Eq. (1) for each realization of $k(\mathbf{x})$, and (iii) obtaining the statistics of these solutions. We also explore an alternative closure of the moment equations for the Kirchhoff transform. This closure assumes that the state variable is a Gaussian random field (or a map of thereof).

The prior Kirchhoff mapping was used earlier to analyze effective properties of gas flow in random media [13]. Since the averaged equations are known to be nonlocal [5,14], such effective properties exist only in a few special cases, such as

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mean uniform flow, where the localization is possible. This paper describes an approach which is applicable to arbitrary flow scenarios.

The Kirchhoff mapping,

$$\Phi[p(\mathbf{x})] = \int_0^p \frac{s\,ds}{\mu(s)Z(s)}, \tag{2}$$

transforms Eq. (1) into a linear stochastic PDE,

$$\nabla \cdot [k(\mathbf{x})\nabla\Phi(\mathbf{x})] = 0. \tag{3}$$

We use the Reynolds decomposition $\mathcal{A} = \langle\mathcal{A}\rangle + \mathcal{A}'$ to represent a random field $\mathcal{A}$ as the sum of its mean, $\langle\mathcal{A}\rangle$, and a zero-mean random fluctuation, $\mathcal{A}'$. Stochastic averaging of the transformed flow equation yields

$$\nabla \cdot [\langle k\rangle\nabla\langle\Phi\rangle - \mathbf{r}] = 0. \tag{4}$$

First, a closure approximation for the cross-product term $\mathbf{r}(\mathbf{x}) \equiv -\langle k'\nabla\Phi'\rangle$ is obtained through the perturbation expansion in σ_Y^2, the variance of log permeability $Y = \ln k$. Instead of using the direct interaction approximation (the Corrsin-like conjecture) [5], we rely on a recursive set of equations for the ith-order terms in the asymptotic series $\langle\Phi\rangle = \langle\Phi^{(0)}\rangle + \langle\Phi^{(1)}\rangle + O(\sigma_Y^4)$ [15]. The superscript (i) denotes terms that contain only ith powers of σ_Y^2. In particular, the zeroth-order approximation, $\langle\Phi^{(0)}\rangle$, is found as the solution of the Laplace equation $\nabla \cdot [k_g\nabla\langle\Phi^{(0)}\rangle] = 0$, where $k_g = \exp(\langle Y\rangle)$ is the geometric mean of k. The first-order approximation, $\langle\Phi^{(1)}\rangle$, is the solution of the Poisson equation $\nabla \cdot [k_g\nabla\langle\Phi^{(1)}\rangle] + f = 0$, where $f = \nabla \cdot [k_g\sigma_Y^2/2\nabla\langle\Phi^{(0)}\rangle] + \mathbf{r}^{(1)}]$ and

$$\mathbf{r}^{(1)} = \int_\Omega k_g C_Y \nabla_{\mathbf{x}}\nabla_{\mathbf{y}}^T G\nabla_{\mathbf{y}}\langle\Phi^{(0)}\rangle d\mathbf{y}. \tag{5}$$

Here integration is over the flow domain Ω, $C_Y(\mathbf{y},\mathbf{x}) = \langle Y'(\mathbf{y})Y'(\mathbf{x})\rangle$ is the two-point covariance function of Y, and $G(\mathbf{y},\mathbf{x})$ is the corresponding zeroth-order mean Green's function. The resulting recursive approximations, together with a similarly derived equation for the first-order approximation of the Kirchhoff transform covariance, are solved by nonlocal finite elements [16].

Note that our perturbation solution for the Kirchhoff transform $\langle\Phi\rangle$ does not require the random field k to be statistically homogeneous, and allows for an arbitrary spatial correlation structure. Unlike closures based on the Corrsin conjecture [5], the recursive approximation does not result in nonlocal, integro-differential equations. Hence, there is no need for localization of Eq. (5).

By way of example, we consider two-dimensional flow in a unit square whose permeability k is a statistically homogeneous, log-normally distributed random field with an exponential covariance function, $C_Y(\mathbf{y},\mathbf{x}) = \sigma_Y^2 \exp(-|\mathbf{y}-\mathbf{x}|/\lambda)$, where λ is the correlation length. The following parameters are used in all subsequent calculations, $\sigma_Y^2 = 1$, $\lambda = 1/12$. Constant pressure is maintained on the lateral boundaries, $p = P_1 = 1$ at $x_1 = 0$ and $p = P_2 = 0$ at $x_1 = 1$. Two other

boundaries, $x_2 = 0$ and $x_2 = 1$ are assumed impermeable. Without loss of generality, we further assume ideal gas [μ = const and $Z(p) = 1$], so that $2\mu\Phi = p^2$, and the conditions on the Dirichlet boundaries become $\Phi = \Phi_1 = 0.5$ at $x_1 = 0$ and $\Phi = \Phi_2 = 0$ at $x_1 = 1$. Note that here and everywhere below we drop μ, so that Φ denotes the renormalized Kirchhoff transform. Φ denotes the Kirchhoff transform normalized by μ.

We check the accuracy of the first-order perturbation solutions for the mean, $\langle\Phi^{[1]}\rangle = \langle\Phi^{(0)}\rangle + \langle\Phi^{(1)}\rangle$, and variance, $[\sigma_\Phi^2]^{[1]}$, of the Kirchhoff transform, Φ, through the comparison with MCS. (The superscript $[i]$ denotes the summation of all terms up to ith power of σ_Y^2.) To insure the stability and accuracy of MCS, we used 4000 realizations of random permeability fields with spatial discretization of $\lambda/4$. This comparison shows an excellent agreement between the two methods, with maximum discrepancies of 0.05% for mean, $\langle\Phi\rangle$ and 1.74% for variance, σ_Φ^2. Note that while our perturbation solutions are formally valid for $\sigma_Y^2 \ll 1$, they remain robust for $\sigma_Y^2 = 1$ used in our example.

Given the moments of the Kirchhoff transform, $\langle\Phi^{[1]}\rangle$ and $[\sigma_\Phi^2]^{[1]}$, the first-order approximation of the mean gas pressure can be obtained as $\langle p^{[1]}\rangle = \langle p^{(0)}\rangle + \langle p^{(1)}\rangle$, where

$$\langle p^{(0)}\rangle^2 = 2\langle\Phi^{(0)}\rangle \tag{6}$$

and

$$\langle p^{(1)}\rangle = \frac{2\langle\Phi^{(0)}\rangle\langle\Phi^{(1)}\rangle - [\sigma_\Phi^2]^{[1]}/2}{(2\langle\Phi^{(0)}\rangle)^{3/2}}. \tag{7}$$

Similarly, the first-order approximation of gas pressure variance is given by

$$[\sigma_p^2]^{[1]} = \frac{[\sigma_\Phi^2]^{[1]}}{2\langle\Phi^{(0)}\rangle}. \tag{8}$$

Alternatively, the mixed moment, $\mathbf{r}$, in Eq. (4) can be derived by assuming that the random state variable Φ is Gaussian [6]. This posterior linear mapping is a special case of mapping closures [11], which assume the state variable to be a function of a Gaussian variable. However, the mapping closures are used in the context of the PDF methods, rather than in the method of moments. Assuming Φ to be Gaussian, leads to the straightforward evaluation of the moments of p. The comparison with MCS shows that the mean and variance of p obtained by means of the Gaussian assumption are as accurate (0.05% discrepancy for the mean and 1.26% discrepancy for the variance) as their counterparts obtained through the perturbation expansion. (The accuracy of our posterior Gaussian mapping suggests that for nonlinear diffusion considered in Ref. [12] one should use the log-normal prior mapping rather than the Gaussian one. Since the two mappings are similar for small values of variance σ_Y^2, it explains why the prior Gaussian mapping of Ref. [12] was accurate for small variances only.) However, as we demon-
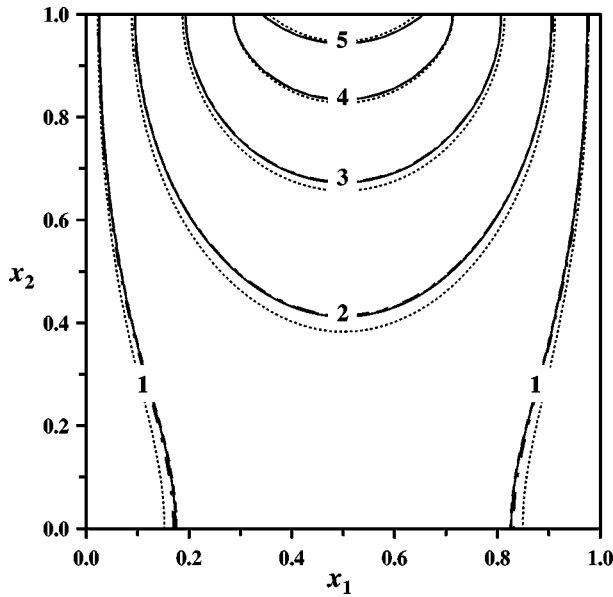
FIG. 1. Mean gas pressure computed by MCS (solid line), the perturbation expansion (dashed line), the linear posterior mapping (dash-dotted line), and the mean-field approximation (dotted line).

strate below, the validity and accuracy of the Gaussian assumption are highly sensitive to the flow scenario and cannot be assessed *a priori*.

To demonstrate this point, we consider a more complicated flow structure. We modify our original example by injecting gas (at the specific rate $q = 1$) through the opening (of width $1/3$) located at the center of the impermeable boundary $x_2 = 1$. Zero pressure is prescribed at the Dirichlet boundaries, $x_1 = 0$ and $x_1 = 1$. The bottom boundary, $x_2 = 0$ is impermeable. Such a flow scenario may serve as an idealized model for the subsurface CO_2 sequestration used to reduce global warming.

The first-order approximations of the mean Kirchhoff transform, $\langle \Phi \rangle$, is in excellent agreement with MCS, with the maximum discrepancy $\leqslant 1\%$. The first-order approximation of the Kirchhoff transform variance, σ_Φ^2, differs by about 25% in the immediate vicinity of the injection area. This discrepancy dissipates rapidly with the distance from the injection interval, where the maximum discrepancy is about 5%. Overall, $[\sigma_\Phi^2]^{[1]}$ captures correctly the qualitative behavior of the Kirchhoff transform variance. It is worthwhile to remember that $[\sigma_\Phi^2]^{[1]}$ represents the lowest-order approximation of gas pressure variance, σ_Φ^2. We expect that evaluating higher-order approximations will improve the accuracy.

Figure 1 compares the mean gas pressure, $\langle p \rangle$, calculated from (i) MCS, (ii) first-order approximations, and (iii) the linear posterior mapping. This comparison shows that both approximations are accurate. The maximum relative error (MRE) between MCS and the perturbation solution is about 0.5%. Once again, this is so despite the fact that the perturbation parameter is relatively high, $\sigma_Y^2 = 1$. MRE for the linear posterior mapping is about 1.2%. In the absence of sources, zeroth-order approximation of mean pressure coin-
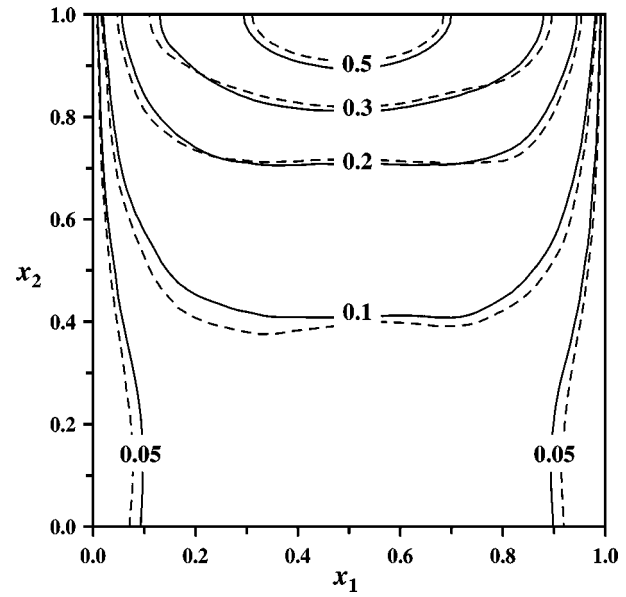
cides with the mean field approximation (the dotted line in Fig. 1). MRE for the mean field approximation is about 6%.

A similar comparison for gas pressure variance is shown in Figs. 2 and 3. While the perturbation solution remains relatively robust, the linear posterior mapping leads to a significant discrepancy with the MCS standard deviation. This discrepancy persists over the whole flow domain. MRE for the perturbation solution is about 20% in the immediate vicinity of the injection interval, and decreases rapidly to 5% away from it. On the other hand, MRE for the linear posterior mapping decays gradually from about 20% in the vicinity of the injection interval to about 15% in the interior part of the flow domain. In the neighborhood of the constant pres-

FIG. 2. Gas pressure variance computed by MCS (solid line) and the perturbation expansion (dashed line).
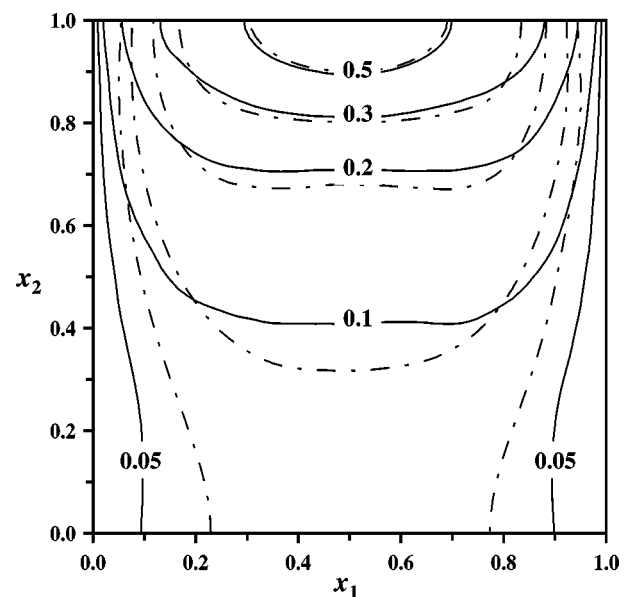

FIG. 3. Gas pressure variance computed by MCS (solid line) and the linear posterior mapping (dash-dotted line).

sure boundaries, MRE exceeds 50%. The relative failure of the posterior linear mapping suggests that it might be necessary to employ nonlinear transformations $\mathcal{T}$, which map a Gaussian random field $X(\mathbf{x})$ onto the random field of state variable, i.e., $p(\mathbf{x}) = \mathcal{T}[X(\mathbf{x})]$.

We used the Kolomogorov test to assess Gaussianity of the empirical distribution of the Kirchhoff transform computed from MCS. The Gaussian hypothesis is rejected at significance levels of 1%, 5%, and 10% for $N = 4000$ Monte Carlo realizations. The difference between the empirical (MCS) and Gaussian distribution exceeds the critical Kolmogorov statistic (for a given significance level) to a different degree throughout the flow domain. Thus, it seems necessary to introduce the space dependency into the posterior mapping closure, $p(\mathbf{x}) = \mathcal{T}[\mathbf{x}, X(\mathbf{x})]$.

The analysis in this paper leads us to the following major conclusions. The prior Kirchhoff mappings, which transform stochastic nonlinear equations similar to Eq. (1) into linear stochastic PDEs, are a useful tool for the moment analysis of such systems. Stochastic averaging of the resulting linear stochastic PDEs with spatially correlated multiplicative noise can be carried out by means of either perturbation expansions or posterior mapping closures. Since Gaussian mapping closures are sensitive to a flow configuration (as specified, for example, by initial, boundary and source functions), the reliance on perturbation expansions seems to be more appealing. This is especially so, since such expansions often remain robust for relatively large variances of the underlying multiplicative noise.

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