

# Direct solution of unsaturated flow in randomly heterogeneous soils

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**ABSTRACT:** We consider steady state unsaturated flow in bounded randomly heterogeneous soils under the influence of random forcing terms. Our aim is to predict pressure heads and fluxes without resorting to Monte Carlo simulation, upscaling or linearization of the constitutive relationship between unsaturated hydraulic conductivity and pressure head. We represent this relationship through Gardner's exponential model, treating its exponent  $\alpha$  as a random constant and saturated hydraulic conductivity,  $K_s$ , as a spatially correlated random field. This allows us to linearize the steady state unsaturated flow equations by means of the Kirchhoff transformation, integrate them in probability space, and obtain exact integro-differential equations for the conditional mean and variance-covariance of transformed pressure head and flux. We solve the latter for flow in the vertical plane, with a point source, by finite elements to second-order of approximation. Our solution compares favorably with conditional Monte Carlo simulations, even for soils that are strongly heterogeneous.

## 1 INTRODUCTION

Saturated hydraulic conductivity and the parameters of constitutive relations between relative conductivity and pressure head in unsaturated soils vary spatially in a manner that cannot be described with certainty. Therefore, they are often modeled as correlated random fields, rendering the corresponding unsaturated flow equations stochastic. If the (geo)statistical properties of these fields can be inferred from measurements, the stochastic flow equations can be solved numerically by conditional Monte Carlo simulation. The corresponding first moments constitute optimum unbiased predictors of quantities such as pressure head and flux. Conditional second moments constitute measures of associated prediction errors. The Monte Carlo method is conceptually straight forward but computationally demanding. It lacks well-established convergence criteria and requires that one specify the probability distribution of the parameter fields.

We present a deterministic alternative to conditional Monte Carlo simulation which allows predicting steady state unsaturated flow under uncertainty, and assess the latter, without having to generate random fields or variables, without upscaling, and without linearizing the constitutive characteristics of the soil. Neuman et al. (1999) and Tartakovsky et al. (1999) have shown that such prediction is possible

when soil properties scale according to the linearly separable model of Vogel et al. (1991). They have demonstrated that when the scaling parameter of pressure head is a random variable independent of location, the steady state unsaturated flow equation can be linearized by means of the Kirchhoff transformation for gravity-free flow. Linearization is also possible in the presence of gravity when hydraulic conductivity varies exponentially with pressure head according to the exponential model of Gardner (1958). This allowed Tartakovsky et al. (1999) to develop exact conditional first- and second-moment equations for unsaturated flow which are nonlocal (integro-differential) and therefore non-Darcian. The authors solved their equations analytically by perturbation for unconditional vertical infiltration. Their solution treats  $\alpha$  as a nonrandom constant and is otherwise valid to second order in the standard deviation,  $\sigma_Y$ , of natural log saturated hydraulic conductivity,  $Y = \ln K_s$ .

Lu (2000) developed perturbation approximations for the nonlocal conditional moment equations of Tartakovsky et al. (1999), valid to second order in both  $\sigma_Y$  and the standard deviation of  $\beta = \ln \alpha$ ,  $\sigma_\beta$ . In this paper, we present only such equations for conditional expectations of pressure head and flux. The equations for conditional second moments can be found in Lu (2000). Based on these approximations, Lu developed a finite element algorithm for flow in the vertical plane when  $Y$  and  $\alpha$  are mutually uncorrelated. We show some of his computational results

for  $\sigma_\beta = 0$  in the presence of a point source, and compare them with those of conditional Monte Carlo simulations.

## 2 STATEMENT OF PROBLEM

We start from the steady state Richards' equation

$$\nabla \cdot [K(\mathbf{x}, \psi) \nabla (\psi(\mathbf{x}) + g x_3)] + f(\mathbf{x}) = 0 \quad \mathbf{x} \in \Omega \quad (1)$$

subject to

$$\psi(\mathbf{x}) = \Psi(\mathbf{x}) \quad \mathbf{x} \in \Gamma_D \quad (2)$$

$$-\mathbf{q}(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N \quad (3)$$

where  $\mathbf{q}$  is flux,  $K$  is unsaturated hydraulic conductivity,  $\psi$  is pressure head,  $g$  is an indicator showing whether the flow is gravity-free or not, being one for flow with gravity and zero for the gravity-free flow,  $x_3$  is the vertical coordinate,  $f$  is a source term,  $\Psi$  is prescribed head on the Dirchlet boundary  $\Gamma_D$ ,  $Q$  is prescribed flux on the Neumann boundary  $\Gamma_N$ , and  $\mathbf{n}$  is a unit outward vector normal to the boundary  $\Gamma$ , the union of  $\Gamma_D$  and  $\Gamma_N$ . All quantities are defined, and measurable, on a bulk support volume  $\omega$  that is small compared to the flow domain  $\Omega$ . The forcing terms  $f$ ,  $\Psi$ ,  $Q$  are random and mutually uncorrelated. This and the fact that  $K$  is a random field renders (1) - (3) stochastic.

According to Gardner's (1958) model

$$K(\mathbf{x}, \psi) = K_s(x) K_r(\mathbf{x}, \psi) \quad K_r(\mathbf{x}, \psi) = e^{\alpha(x)\psi(x)} \quad (4)$$

where  $K_r$  is relative conductivity and  $\alpha$  is a positive exponent. Setting  $\alpha = \text{constant}$  allows defining the Kirchhoff transformation (Tartakovsky et al., 1999)

$$\Phi(\mathbf{x}) = \int_{-\infty}^{\psi(\mathbf{x})} K_r(\xi) d\xi = \int_{-\infty}^{\psi(\mathbf{x})} e^{\alpha\xi} d\xi = \frac{1}{\alpha} e^{\alpha\psi(\mathbf{x})} \quad (5)$$

which transforms (1) - (3) into

$$\nabla \cdot [K_s(\mathbf{x}) (\nabla \Phi(\mathbf{x}) + g \alpha \Phi(\mathbf{x}) \mathbf{e}_3)] + f(\mathbf{x}) = 0 \quad \mathbf{x} \in \Omega \quad (6)$$

$$\Phi(\mathbf{x}) = H(\mathbf{x}), \quad H(\mathbf{x}) = \frac{1}{\alpha} e^{\alpha\Psi(\mathbf{x})} \quad \mathbf{x} \in \Gamma_D \quad (7)$$

$$\mathbf{n}(\mathbf{x}) \cdot [K_s(\mathbf{x}) (\nabla \Phi(\mathbf{x}) + g \alpha \Phi(\mathbf{x}) \mathbf{e}_3)] = Q(\mathbf{x}) \quad \mathbf{x} \in \Gamma_N \quad (8)$$

where  $\mathbf{e}_3 = (0, 0, 1)^T$ .

## 3 EXACT CONDITIONAL MEAN EQUATIONS

### 3.1 Exact equations for $\langle \Phi(\mathbf{x}) \rangle$

We write

$$\begin{aligned} \mathbf{K}_s(\mathbf{x}) &= \langle \mathbf{K}_s(\mathbf{x}) \rangle + \mathbf{K}'_s(\mathbf{x}) & \langle \mathbf{K}'_s(\mathbf{x}) \rangle &\equiv 0 \\ \Phi(\mathbf{x}) &= \langle \Phi(\mathbf{x}) \rangle + \Phi'(\mathbf{x}) & \langle \Phi'(\mathbf{x}) \rangle &\equiv 0 \\ \alpha &= \langle \alpha \rangle + \alpha' & \langle \alpha' \rangle &\equiv 0 \end{aligned} \quad (9)$$

where  $\langle \cdot \rangle$  indicates conditional mean and primed quantities define zero mean random fluctuations about the mean. Substituting (9) into (6) - (8) and taking their conditional mean yields

$$\begin{cases} \nabla \cdot [ \langle K_s(\mathbf{x}) \rangle \nabla \langle \Phi(\mathbf{x}) \rangle - \mathbf{r}(\mathbf{x}) \\ + g ( \langle \alpha \rangle \langle K_s(\mathbf{x}) \rangle \langle \Phi(\mathbf{x}) \rangle + \langle \alpha \rangle R_{K\Phi}(\mathbf{x}) \\ + \langle K_s(\mathbf{x}) \rangle R_{\alpha\Phi}(\mathbf{x}) + R_{\alpha K\Phi}(\mathbf{x}) ) \mathbf{e}_3 ] + \langle f(\mathbf{x}) \rangle = 0 & \mathbf{x} \in \Omega \\ \langle \Phi(\mathbf{x}) \rangle = \langle H(\mathbf{x}) \rangle & \mathbf{x} \in \Gamma_D \\ \mathbf{n}(\mathbf{x}) \cdot [*] = \langle Q(\mathbf{x}) \rangle & \mathbf{x} \in \Gamma_N \end{cases} \quad (10)$$

where  $[*]$  is identical to the other term in [ ] and

$$\begin{aligned} \mathbf{r}(\mathbf{x}) &= -\langle K'_s(\mathbf{x}) \nabla \Phi'(\mathbf{x}) \rangle \\ R_{K\Phi}(\mathbf{x}) &= \langle K'_s(\mathbf{x}) \Phi'(\mathbf{x}) \rangle \\ R_{\alpha\Phi}(\mathbf{x}) &= \langle \alpha' \Phi'(\mathbf{x}) \rangle \\ R_{\alpha K\Phi}(\mathbf{x}) &= \langle \alpha' K'(\mathbf{x}) \Phi'(\mathbf{x}) \rangle \end{aligned} \quad (11)$$

Substituting (9) into (6) - (8) and subtracting (10) gives

$$\begin{cases} \nabla \cdot [ K_s(\mathbf{x}) \nabla \Phi'(\mathbf{x}) + K'_s(\mathbf{x}) \nabla \langle \Phi(\mathbf{x}) \rangle + \mathbf{r}(\mathbf{x}) \\ + g ( \alpha K_s(\mathbf{x}) \Phi'(\mathbf{x}) + \alpha' K_s(\mathbf{x}) \langle \Phi(\mathbf{x}) \rangle \\ + \langle \alpha \rangle K'_s(\mathbf{x}) \langle \Phi(\mathbf{x}) \rangle - \langle \alpha \rangle R_{K\Phi}(\mathbf{x}) - \langle K_s(\mathbf{x}) \rangle R_{\alpha\Phi}(\mathbf{x}) \\ - R_{\alpha K\Phi}(\mathbf{x}) ) \mathbf{e}_3 ] + f'(\mathbf{x}) = 0 & \mathbf{x} \in \Omega \\ \Phi'(\mathbf{x}) = H'(\mathbf{x}) & \mathbf{x} \in \Gamma_D \\ \mathbf{n}(\mathbf{x}) \cdot [*] = Q'(\mathbf{x}) & \mathbf{x} \in \Gamma_N \end{cases} \quad (12)$$

Let  $G(\mathbf{y}, \mathbf{x})$  be an auxiliary function that satisfies

$$\begin{cases} \nabla_{\mathbf{y}} \cdot [ K_s(\mathbf{y}) \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) ] - g \alpha \mathbf{e}_3^T K_s(\mathbf{y}) \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) \\ + \delta(\mathbf{x} - \mathbf{y}) = 0 & \mathbf{x}, \mathbf{y} \in \Omega \\ G(\mathbf{y}, \mathbf{x}) = 0 & \mathbf{x} \in \Omega, \mathbf{y} \in \Gamma_D \\ K_s(\mathbf{y}) \nabla_{\mathbf{y}} G(\mathbf{y}, \mathbf{x}) \cdot \mathbf{n}(\mathbf{y}) = 0 & \mathbf{x} \in \Omega, \mathbf{y} \in \Gamma_N \end{cases} \quad (13)$$

Rewriting (12) in terms of  $\mathbf{y}$ , multiplying by  $G$  and integrating with respect to  $\mathbf{y}$  over  $\Omega$  yields

$$\begin{aligned}
& \Phi'(\mathbf{x}) \\
&= -\int_{\Omega} \nabla_y^T G(\mathbf{y}, \mathbf{x}) \left[ K'_s(\mathbf{y}) \nabla \langle \Phi(\mathbf{y}) \rangle + \mathbf{r}(\mathbf{y}) \right. \\
&\quad + g \left( \alpha' K'_s(\mathbf{y}) \langle \Phi(\mathbf{y}) \rangle + \langle \alpha \rangle K'_s(\mathbf{y}) \langle \Phi(\mathbf{y}) \rangle \right. \\
&\quad \left. \left. - \langle \alpha \rangle R_{K\Phi}(\mathbf{y}) - \langle K_s(\mathbf{y}) \rangle R_{\alpha\Phi}(\mathbf{y}) - R_{\alpha K\Phi}(\mathbf{y}) \right) \mathbf{e}_3 \right] d\Omega \\
&+ \int_{\Omega} f'(\mathbf{y}) G(\mathbf{y}, \mathbf{x}) d\Omega \\
&+ \int_{\Gamma_N} G(\mathbf{y}, \mathbf{x}) Q'(\mathbf{y}) d\Gamma \\
&- \int_{\Gamma_D} H'(\mathbf{y}) K_s(\mathbf{y}) \nabla_y G(\mathbf{y}, \mathbf{x}) \cdot \mathbf{n}(\mathbf{y}) d\Gamma
\end{aligned} \tag{14}$$

This allows developing explicit integral expressions for all four terms in (11), for example

$$\begin{aligned}
\mathbf{r}(\mathbf{x}) &= -\langle K'_s(\mathbf{x}) \nabla \Phi'(\mathbf{x}) \rangle \\
&= \int_{\Omega} \langle K'_s(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}) K'_s(\mathbf{y}) \rangle \nabla \langle \Phi(\mathbf{y}) \rangle d\Omega \\
&+ \int_{\Omega} \langle K'_s(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}) \rangle \mathbf{r}(\mathbf{y}) d\Omega \\
&+ g \langle \alpha \rangle \int_{\Omega} \langle K'_s(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}) K'_s(\mathbf{y}) \rangle \langle \Phi(\mathbf{y}) \rangle \mathbf{e}_3 d\Omega \\
&+ g \int_{\Omega} \langle \alpha' K'_s(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}) K_s(\mathbf{y}) \rangle \langle \Phi(\mathbf{y}) \rangle \mathbf{e}_3 d\Omega \\
&- g \int_{\Omega} \langle K'_s(\mathbf{x}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}) \rangle \\
&\quad * \left( \langle \alpha \rangle R_{K\Phi}(\mathbf{y}) + \langle K_s(\mathbf{y}) \rangle R_{\alpha\Phi}(\mathbf{y}) + R_{\alpha K\Phi}(\mathbf{y}) \right) \mathbf{e}_3 d\Omega \\
&+ \int_{\Gamma_D} \langle K'_s(\mathbf{x}) H'(\mathbf{y}) \nabla_x \nabla_y^T G(\mathbf{y}, \mathbf{x}) K'_s(\mathbf{y}) \rangle \mathbf{n}(\mathbf{y}) d\Gamma
\end{aligned} \tag{15}$$

The integral over  $\Gamma_N$  and that containing  $f'$  have been omitted because  $K'_s$  and  $G$  are independent of  $Q'$  and  $f'$ . The integral over  $\Gamma_D$  remains because both  $H'$  and  $G'$  depend on  $\alpha'$ .

### 3.2 Exact expression for $\langle \mathbf{q}(\mathbf{x}) \rangle$

By virtue of (6) and (7), Darcy's law transforms into

$$\mathbf{q}(\mathbf{x}) = -\mathbf{K}_s(\mathbf{x}) [\nabla \Phi(\mathbf{x}) + g\alpha\Phi(\mathbf{x}) \mathbf{e}_3] \tag{16}$$

Writing  $\mathbf{q}(\mathbf{x}) = \langle \mathbf{q}(\mathbf{x}) \rangle + \mathbf{q}'(\mathbf{x})$ , substituting (9) into (16), and taking conditional mean, we obtain an exact expression for the conditional mean flux  $\langle \mathbf{q}(\mathbf{x}) \rangle$ ,

$$\begin{aligned}
\langle \mathbf{q}(\mathbf{x}) \rangle &= -\langle \mathbf{K}_s(\mathbf{x}) \rangle \nabla \langle \Phi(\mathbf{x}) \rangle + \mathbf{r}(\mathbf{x}) \\
&+ g \langle \mathbf{K}_s(\mathbf{x}) \rangle \left( \langle \alpha \rangle \langle \Phi(\mathbf{x}) \rangle + R_{\alpha\Phi}(\mathbf{x}) \right) \mathbf{e}_3 \\
&- g \left( \langle \alpha \rangle R_{K\Phi}(\mathbf{x}) + R_{\alpha K\Phi}(\mathbf{x}) \right) \mathbf{e}_3
\end{aligned} \tag{17}$$

where  $\mathbf{R}_{\alpha\Phi}(\mathbf{x})$ ,  $\mathbf{R}_{K\Phi}(\mathbf{x})$ ,  $\mathbf{R}_{\alpha K\Phi}(\mathbf{x})$  are defined in (11).

## 4 RECURSIVE CONDITIONAL MEAN FLOW APPROXIMATIONS

The above conditional mean equations are exact but not workable because they include a number of unknown moments. To render them workable, we expand them in powers of  $\sigma_Y$  and  $\sigma_\beta$ , which represent measures of the standard deviation of  $Y'(\mathbf{x})$  and  $\beta'$ , respectively. For example,

$$\begin{aligned}
\langle \Phi(\mathbf{x}) \rangle &= \sum_{n,m=0}^{\infty} \langle \Phi^{(n,m)}(\mathbf{x}) \rangle \\
\langle K_s(\mathbf{x}) \rangle &= \langle e^{\langle Y \rangle + Y'} \rangle = K_G(\mathbf{x}) \sum_{n=0}^{\infty} \frac{\langle Y'^n \rangle}{n!} \\
\langle \alpha \rangle &= \langle e^{\langle \beta \rangle + \beta'} \rangle = \alpha_G \sum_{m=0}^{\infty} \frac{\langle \beta'^m \rangle}{m!}
\end{aligned} \tag{18}$$

where  $(n,m)$  designates terms including  $n^{\text{th}}$  power of  $\sigma_Y$  and  $m^{\text{th}}$  power of  $\sigma_\beta$ , and  $K_G$  and  $\alpha_G$  are geometric mean values of  $K$  and  $\alpha$ , respectively. The expansion is not guaranteed to be valid for strongly heterogeneous soils with  $\sigma_Y \geq 1$  and  $\sigma_\beta \geq 1$ . As we shall see, it actually works well for relatively large values of  $\sigma_Y$  as long as  $\sigma_\beta$  remains small.

### 4.1 Recursive approximations for $\langle \Phi(\mathbf{x}) \rangle$

Expansion of (10) to second order in  $\sigma_Y$  and  $\sigma_\beta$  yields the following set of recursive equations,

$$\begin{cases} \nabla \cdot \left[ K_G(\mathbf{x}) \left( \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle + g\alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \mathbf{e}_3 \right) \right] \\ \quad + \langle f(\mathbf{x}) \rangle = 0 & \mathbf{x} \in \Omega \\ \langle \Phi^{(0,0)}(\mathbf{x}) \rangle = \langle H^{(0,0)}(\mathbf{x}) \rangle & \mathbf{x} \in \Gamma_D \\ \mathbf{n}(\mathbf{x}) \cdot [*] = \langle Q(\mathbf{x}) \rangle & \mathbf{x} \in \Gamma_N \end{cases} \tag{19}$$

$$\begin{cases} \nabla \cdot \left[ K_G(\mathbf{x}) \nabla \langle \Phi^{(0,2)}(\mathbf{x}) \rangle + gK_G(\mathbf{x}) \left( \alpha_G \langle \Phi^{(0,2)}(\mathbf{x}) \rangle \right. \right. \\ \quad \left. \left. + 0.5\alpha_G\sigma_\beta^2 \langle \Phi^{(0,0)}(\mathbf{x}) \rangle + R_{\alpha\Phi}^{(0,2)}(\mathbf{x}) \right) \mathbf{e}_3 \right] = 0 & \mathbf{x} \in \Omega \\ \langle \Phi^{(0,2)}(\mathbf{x}) \rangle = \langle H^{(0,2)}(\mathbf{x}) \rangle & \mathbf{x} \in \Gamma_D \\ \mathbf{n}(\mathbf{x}) \cdot [*] = 0 & \mathbf{x} \in \Gamma_N \end{cases} \tag{20}$$

$$\begin{cases} \nabla \cdot \left[ K_G(\mathbf{x}) \left( \nabla \langle \Phi^{(2,0)}(\mathbf{x}) \rangle + 0.5\sigma_Y^2(\mathbf{x}) \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) \right. \\ \quad \left. - \mathbf{r}^{(2,0)}(\mathbf{x}) + g \left( \alpha_G K_G(\mathbf{x}) \left( \langle \Phi^{(2,0)}(\mathbf{x}) \rangle \right. \right. \right. \\ \quad \left. \left. + 0.5\sigma_Y^2(\mathbf{x}) \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) + \alpha_G R_{K\Phi}^{(2,0)}(\mathbf{x}) \right) \mathbf{e}_3 \right] = 0 & \mathbf{x} \in \Omega \\ \langle \Phi^{(2,0)}(\mathbf{x}) \rangle = 0 & \mathbf{x} \in \Gamma_D \\ \mathbf{n}(\mathbf{x}) \cdot [*] = 0 & \mathbf{x} \in \Gamma_N \end{cases} \tag{21}$$

$$\left. \begin{aligned}
& \nabla \cdot \left\{ K_G(\mathbf{x}) \left( \nabla \langle \Phi^{(2,2)}(\mathbf{x}) \rangle + \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle \Phi^{(0,2)}(\mathbf{x}) \rangle \right) \right. \\
& - \mathbf{r}^{(2,2)}(\mathbf{x}) \\
& + g \left[ \alpha_G K_G(\mathbf{x}) \left( \langle \Phi^{(2,2)}(\mathbf{x}) \rangle + \frac{\sigma_\beta^2}{2} \langle \Phi^{(2,0)}(\mathbf{x}) \rangle \right. \right. \\
& \quad \left. \left. + \frac{\sigma_Y^2(\mathbf{x})}{2} \langle \Phi^{(0,2)}(\mathbf{x}) \rangle + \frac{\sigma_\beta^2 \sigma_Y^2(\mathbf{x})}{4} \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) \right. \\
& + \alpha_G \left( R_{K\Phi}^{(2,2)}(\mathbf{x}) + \frac{\sigma_\beta^2}{2} R_{K\Phi}^{(2,0)}(\mathbf{x}) \right) + R_{\alpha K\Phi}^{(2,2)}(\mathbf{x}) \\
& \left. + K_G(\mathbf{x}) \left( R_{\alpha\Phi}^{(2,2)}(\mathbf{x}) + \frac{\sigma_Y^2(\mathbf{x})}{2} R_{\alpha\Phi}^{(0,2)}(\mathbf{x}) \right) \right] \mathbf{e}_3 \Big\} = 0 \quad \mathbf{x} \in \Omega \\
& \langle \Phi^{(2,2)}(\mathbf{x}) \rangle = 0 \quad \mathbf{x} \in \Gamma_D \\
& \mathbf{n}(\mathbf{x}) \cdot [*] = 0 \quad \mathbf{x} \in \Gamma_N
\end{aligned} \right\} \quad (22)$$

where  $\langle H^{(0,0)} \rangle$  and  $\langle H^{(0,2)} \rangle$  can be derived from perturbation expansion of (7). All terms  $\langle \Phi^{(n,m)}(\mathbf{x}) \rangle$  with  $n$  or  $m$  equal to 1 are zero. To illustrate how terms are evaluated recursively to second order, we present the corresponding nonzero expressions for  $\mathbf{r}$ ,

$$\begin{aligned}
& \mathbf{r}^{(2,0)}(\mathbf{x}) \\
& = \int_{\Omega} K_G(\mathbf{x}) C_Y(\mathbf{x}, \mathbf{y}) \nabla_x \nabla_y^T G^{(0,0)}(\mathbf{y}, \mathbf{x}) K_G(\mathbf{y}) \\
& \quad * \left( \nabla \langle \Phi^{(0,0)}(\mathbf{y}) \rangle + g \alpha_G \langle \Phi^{(0,0)}(\mathbf{y}) \rangle \mathbf{e}_3 \right) d\Omega \quad (23)
\end{aligned}$$

$$\begin{aligned}
& \mathbf{r}^{(2,2)}(\mathbf{x}) \\
& = \int_{\Omega} K_G(\mathbf{x}) C_Y(\mathbf{x}, \mathbf{y}) \nabla_x \nabla_y^T \langle G^{(0,2)}(\mathbf{y}, \mathbf{x}) \rangle K_G(\mathbf{y}) \\
& \quad * \left[ \nabla \langle \Phi^{(0,0)}(\mathbf{y}) \rangle + g \alpha_G \langle \Phi^{(0,0)}(\mathbf{y}) \rangle \mathbf{e}_3 \right] d\Omega \\
& + \int_{\Omega} K_G(\mathbf{x}) C_Y(\mathbf{x}, \mathbf{y}) \nabla_x \nabla_y^T G^{(0,0)}(\mathbf{y}, \mathbf{x}) K_G(\mathbf{y}) \left[ \nabla \langle \Phi^{(0,2)}(\mathbf{y}) \rangle \right. \\
& \quad \left. + g \alpha_G \left( \langle \Phi^{(0,2)}(\mathbf{y}) \rangle + 0.5 \sigma_\beta^2 \langle \Phi^{(0,0)}(\mathbf{y}) \rangle \right) \mathbf{e}_3 \right] d\Omega \\
& + g \alpha_G \int_{\Omega} K_G(\mathbf{x}) \left[ C_Y(\mathbf{x}, \mathbf{y}) \langle \beta' \nabla_x \nabla_y^T G^{(0,1)}(\mathbf{y}, \mathbf{x}) \rangle \right. \\
& \quad \left. + \langle \beta' Y'(\mathbf{x}) \nabla_x \nabla_y^T G^{(1,1)}(\mathbf{y}, \mathbf{x}) \rangle \right] K_G(\mathbf{y}) \langle \Phi^{(0,0)}(\mathbf{y}) \rangle \mathbf{e}_3 d\Omega \\
& - g \int_{\Omega} K_G(\mathbf{x}) \langle Y'(\mathbf{x}) \nabla_x \nabla_y^T G^{(1,0)}(\mathbf{y}, \mathbf{x}) \rangle K_G(\mathbf{y}) R_{\alpha\Phi}^{(0,2)}(\mathbf{y}) d\Omega
\end{aligned} \quad (24)$$

Evaluating  $\langle \Phi \rangle$  to second order requires 1) solving (19) for  $\langle \Phi^{(0,0)} \rangle$  and (13) for  $G^{(0,0)}$  (upon replacing  $K_s$  and  $\alpha$  in (13) by  $K_G$  and  $\alpha_G$ ); 2) evaluating moments that involve  $G$  up to first order, such as  $\langle \beta' G^{(0,1)} \rangle$  and  $\langle Y' G^{(1,0)} \rangle$ ; 3) evaluating the moments in (11) up to second order in one of the expansion parameters, for example  $\mathbf{r}^{(2,0)}$ ,  $R_{\alpha\Phi}^{(0,2)}$ ,  $R_{K\Phi}^{(2,0)}$ ; 4) solving (20) - (21) for  $\langle \Phi^{(0,2)} \rangle$  and  $\langle \Phi^{(2,0)} \rangle$ , respectively; 5) evaluating  $\mathbf{r}^{(2,2)}$ ,  $R_{\alpha\Phi}^{(2,2)}$ ,  $R_{K\Phi}^{(2,2)}$ ,  $R_{\alpha K\Phi}^{(2,2)}$ ; and 6) solving (22) for  $\langle \Phi^{(2,2)} \rangle$ . A detailed derivation of all the requisite equations is given by Lu (2000).

#### 4.2 Recursive approximations of $\langle \mathbf{q}(\mathbf{x}) \rangle$

Expansion of (17) leads to the following recursive approximations of  $\langle \mathbf{q}(\mathbf{x}) \rangle$  to second order,

$$\begin{aligned}
& \langle \mathbf{q}^{(0,0)}(\mathbf{x}) \rangle \\
& = -K_G(\mathbf{x}) \left( \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle + g \alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \mathbf{e}_3 \right) \quad \mathbf{x} \in \Omega \quad (25)
\end{aligned}$$

$$\begin{aligned}
& \langle \mathbf{q}^{(2,0)}(\mathbf{x}) \rangle \\
& = -K_G(\mathbf{x}) \left[ \nabla \langle \Phi^{(2,0)}(\mathbf{x}) \rangle + \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right. \\
& \quad \left. + g \alpha_G \left( \langle \Phi^{(2,0)}(\mathbf{x}) \rangle + \frac{\sigma_Y^2(\mathbf{x})}{2} \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) \mathbf{e}_3 \right] \\
& \quad + \mathbf{r}^{(2,0)}(\mathbf{x}) - g \alpha_G R_{K\Phi}^{(2,0)}(\mathbf{x}) \mathbf{e}_3 \quad \mathbf{x} \in \Omega \quad (26)
\end{aligned}$$

$$\begin{aligned}
& \langle \mathbf{q}^{(0,2)}(\mathbf{x}) \rangle \\
& = -K_G(\mathbf{x}) \left[ \nabla \langle \Phi^{(0,2)}(\mathbf{x}) \rangle + g \alpha_G \langle \Phi^{(0,2)}(\mathbf{x}) \rangle \mathbf{e}_3 \right. \\
& \quad \left. + g \left( 0.5 \alpha_G \sigma_\beta^2 \langle \Phi^{(0,2)}(\mathbf{x}) \rangle + R_{\alpha\Phi}^{(0,2)}(\mathbf{x}) \right) \mathbf{e}_3 \right] \quad (27)
\end{aligned}$$

$$\begin{aligned}
& \langle \mathbf{q}^{(2,2)}(\mathbf{x}) \rangle \\
& = -K_G(\mathbf{x}) \left[ \nabla \langle \Phi^{(2,2)}(\mathbf{x}) \rangle + \frac{\sigma_Y^2(\mathbf{x})}{2} \nabla \langle \Phi^{(0,2)}(\mathbf{x}) \rangle \right. \\
& \quad \left. + g \alpha_G \left( \langle \Phi^{(2,2)}(\mathbf{x}) \rangle + \frac{\sigma_\beta^2}{2} \langle \Phi^{(2,0)}(\mathbf{x}) \rangle \right. \right. \\
& \quad \left. \left. + \frac{\sigma_Y^2(\mathbf{x})}{2} \left( \langle \Phi^{(0,2)}(\mathbf{x}) \rangle + \frac{\sigma_\beta^2}{2} \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) \right) \right] \mathbf{e}_3 \\
& + g \left( R_{\alpha\Phi}^{(2,2)}(\mathbf{x}) + \frac{\sigma_Y^2(\mathbf{x})}{2} R_{\alpha\Phi}^{(0,2)}(\mathbf{x}) \right) \mathbf{e}_3 - \mathbf{r}^{(2,2)}(\mathbf{x}) \\
& + g \left[ \alpha_G \left( R_{K\Phi}^{(2,2)}(\mathbf{x}) + \frac{\sigma_Y^2(\mathbf{x})}{2} R_{K\Phi}^{(0,2)}(\mathbf{x}) \right) + R_{\alpha K\Phi}^{(2,2)}(\mathbf{x}) \right] \mathbf{e}_3 \quad (28)
\end{aligned}$$

### 5 FINITE ELEMENT ALGORITHM

In most cases of practical interest, conditioning points are sparse enough to ensure that conditional mean quantities vary more slowly in space than do their random counterparts. Hence one can resolve the former (by an algorithm such as we propose) on a coarser grid than is required to resolve the latter (by Monte Carlo simulation). Here we nevertheless use a fine grid to allow comparing our direct finite element solution of the recursive moment equations with a finite element Monte Carlo solution of the original stochastic flow equations.

We solve the recursive conditional moment equations by a Galerkin finite element scheme on a rectangular vertical grid with square elements, using bilinear weight functions  $\xi_n(\mathbf{x})$ . For simplicity, we consider only deterministic forcing terms. To illustrate our approach we consider the Galerkin orthogonalization of (19) which, following the application of Green's first identity, yields

$$\begin{aligned} & \int_{\Omega} K_G(\mathbf{x}) \left( \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle + g \alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \mathbf{e}_3 \right) \cdot \nabla \xi_n(\mathbf{x}) d\Omega \\ &= \int_{\Gamma_D} K_G(\mathbf{x}) \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \xi_n(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\Gamma \\ &+ \int_{\Gamma_N} \langle Q(\mathbf{x}) \rangle \xi_n(\mathbf{x}) d\Gamma + \int_{\Omega} \langle f(\mathbf{x}) \rangle \xi_n(\mathbf{x}) d\Omega \quad \mathbf{x} \in \Omega \end{aligned} \quad (29)$$

where  $n = 1, 2, \dots, NN$ ,  $NN$  being the number of nodes. Let

$$\langle \Phi^{(0,0)}(\mathbf{x}) \rangle = \sum_{m=1}^{NN} \langle \Phi_m^{(0,0)} \rangle \xi_m(\mathbf{x}) \quad (30)$$

where  $\langle \Phi_m^{(0,0)} \rangle$  is  $\langle \Phi^{(0,0)}(\mathbf{x}) \rangle$  evaluated at node  $m$ . Substituting (30) into the leftmost integral in (29), and defining the matrix components

$$\begin{aligned} A_{nm} &= \sum_e A_{nm}^{(e)} = \int_{\Omega} K_G(\mathbf{x}) \nabla \xi_n(\mathbf{x}) \cdot \nabla \xi_m(\mathbf{x}) d\Omega \\ B_{nm} &= \sum_e B_{nm}^{(e)} = \mathbf{e}_3^T \int_{\Omega} K_G(\mathbf{x}) \xi_n(\mathbf{x}) \nabla \xi_m(\mathbf{x}) d\Omega \end{aligned} \quad (31)$$

(29) becomes

$$\begin{aligned} & \sum_{m=1}^{NN} (A_{nm} + g \alpha_G B_{nm}) \langle \Phi_m^{(0,0)} \rangle \\ &= \int_{\Gamma_D} K_G(\mathbf{x}) \nabla \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \xi_n(\mathbf{x}) \cdot \mathbf{n}(\mathbf{x}) d\Gamma \\ &+ \int_{\Gamma_N} \langle Q(\mathbf{x}) \rangle \xi_n(\mathbf{x}) d\Gamma \\ &+ \int_{\Omega} \langle f(\mathbf{x}) \rangle \xi_n(\mathbf{x}) d\Omega \quad n = 1, 2, \dots, NN; \mathbf{x} \in \Omega \end{aligned} \quad (32)$$

Equations corresponding to  $n \notin \Gamma_D$  can be dropped; at all other nodes, the integral over  $\Gamma_D$  vanishes. As all terms on the right-hand-side are known, the corresponding integrals can be evaluated numerically and (32) solved for  $\langle \Phi^{(0,0)}(\mathbf{x}) \rangle$  at all nodes.

To illustrate how the moments in (11) are evaluated numerically, consider for example  $\mathbf{r}^{(2,0)}(\mathbf{x})$ . For any  $\mathbf{x} \in e$  and  $\mathbf{y} \in e'$  in elements  $e$  and  $e'$ , let

$$\langle G^{(0,0)(e',e)}(\mathbf{y}, \mathbf{x}) \rangle = \sum_{j=1}^N \sum_{k=1}^N G_{jk}^{(0,0)(e',e)} \xi_j^{(e')}(\mathbf{y}) \xi_k^{(e)}(\mathbf{x}) \quad (33)$$

$$\langle \Phi^{(0,0)(e')}(\mathbf{y}) \rangle = \sum_{p=1}^N \langle \Phi_p^{(0,0)(e')} \rangle \xi_p^{(e')}(\mathbf{y}) \quad (34)$$

where  $G_{jk}^{(0,0)(e',e)}$  is  $G^{(0,0)}$  associated with local node  $j$  in element  $e'$  and node  $k$  in element  $e$ ,  $\langle \Phi_p^{(0,0)(e')} \rangle$  is

$\langle \Phi^{(0,0)}(\mathbf{x}) \rangle$  at local node  $p$  in element  $e'$ ,  $N$  is the number of nodes in an element,  $\xi_k^{(e)}$  is  $\xi$  associated with local node  $k$  in element  $e$ , and  $\xi_j^{(e')}$  is  $\xi$  associated with local node  $j$  in element  $e'$ . Substituting (33) and (34) into (23), and writing the integral over  $\Omega$  as a sum of integrals over elements,

$$\begin{aligned} & \mathbf{r}^{(2,0)(e)}(\mathbf{x}) \\ &= \sum_{e'} C_Y(e, e') K_G^{(e)}(\mathbf{x}) \sum_{j=1}^N \sum_{k=1}^N \sum_{p=1}^N G_{jk}^{(0,0)(e',e)} \langle \Phi_p^{(0,0)(e')} \rangle \\ & \quad * (A_{jp}^{(e')} + g \alpha_G B_{pj}^{(e')}) \nabla \xi_k^{(e)}(\mathbf{x}) \end{aligned} \quad (38)$$

where  $C_Y(e, e')$  is autocovariance of  $Y'$  between elements  $e$  and  $e'$ , and

$$\begin{aligned} A_{jp}^{(e')} &= \int_{\Omega_{e'}} \nabla^T \xi_j^{(e')}(\mathbf{y}) K_G^{(e')}(\mathbf{y}) \nabla \xi_p^{(e')}(\mathbf{y}) d\Omega \quad j, p = \overline{1, N} \\ B_{pj}^{(e')} &= \int_{\Omega_{e'}} \nabla^T \xi_j^{(e')}(\mathbf{y}) K_G^{(e')}(\mathbf{y}) \xi_p^{(e')}(\mathbf{y}) \mathbf{e}_2 d\Omega \quad j, p = \overline{1, N} \end{aligned} \quad (39)$$

## 6 MEAN PRESSURE HEAD

Once the problem has been solved in terms of Kirchhoff-transformed pressure head, it can be back-transformed to yield, with the aid of (5),

$$\langle \Psi^{(0,0)}(\mathbf{x}) \rangle = \frac{1}{\alpha_G} \ln \left( \alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) \quad (40)$$

$$\begin{aligned} & \langle \Psi^{(0,2)}(\mathbf{x}) \rangle = -\frac{\sigma_{\beta}^2}{\alpha_G} + \frac{\sigma_{\beta}^2}{2\alpha_G} \ln \left( \alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle \right) \\ & + \frac{1}{\alpha_G} \left[ \frac{\langle \Phi^{(0,2)}(\mathbf{x}) \rangle}{\langle \Phi^{(0,0)}(\mathbf{x}) \rangle} - \frac{R_{\alpha\Phi}^{(0,2)}(\mathbf{x})}{\alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle} - \frac{C_{\Phi}^{(0,2)}(\mathbf{x}, \mathbf{x})}{2 \langle \Phi^{(0,0)}(\mathbf{x}) \rangle^2} \right] \end{aligned} \quad (41)$$

$$\langle \Psi^{(2,0)}(\mathbf{x}) \rangle = \frac{1}{\alpha_G} \left[ \frac{\langle \Phi^{(2,0)}(\mathbf{x}) \rangle}{\langle \Phi^{(0,0)}(\mathbf{x}) \rangle} - \frac{1}{2} \frac{C_{\Phi}^{(2,0)}(\mathbf{x}, \mathbf{x})}{\langle \Phi^{(0,0)}(\mathbf{x}) \rangle^2} \right] \quad (42)$$

$$\begin{aligned} & \langle \Psi^{(2,2)}(\mathbf{x}) \rangle = \frac{1}{\alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle} \left[ \langle \Phi^{(2,2)}(\mathbf{x}) \rangle \right. \\ & \quad \left. - \frac{\langle \Phi^{(2,0)}(\mathbf{x}) \rangle \langle \Phi^{(0,2)}(\mathbf{x}) \rangle}{\langle \Phi^{(0,0)}(\mathbf{x}) \rangle} - \frac{C_{\Phi}^{(2,2)}(\mathbf{x}, \mathbf{x})}{2 \langle \Phi^{(0,0)}(\mathbf{x}) \rangle} \right] \\ & - \frac{\sigma_{\beta}^2}{2\alpha_G \langle \Phi^{(0,0)}(\mathbf{x}) \rangle} \left[ \langle \Phi^{(2,0)}(\mathbf{x}) \rangle - \frac{C_{\Phi}^{(2,0)}(\mathbf{x}, \mathbf{x})}{2 \langle \Phi^{(0,0)}(\mathbf{x}) \rangle} \right] \\ & - \frac{1}{\alpha_G^2 \langle \Phi^{(0,0)}(\mathbf{x}) \rangle} \left[ R_{\alpha\Phi}^{(2,2)}(\mathbf{x}) - \frac{R_{\alpha\Phi}^{(0,2)}(\mathbf{x}) \langle \Phi^{(2,0)}(\mathbf{x}) \rangle}{\langle \Phi^{(0,0)}(\mathbf{x}) \rangle} \right] \end{aligned} \quad (43)$$

where  $C_{\Phi}$  is the covariance of  $\Phi$ . The mean pressure head is given to second order by

$$\begin{aligned} & \langle \psi^{[2,2]}(\mathbf{x}) \rangle \\ &= \langle \psi^{(0,0)}(\mathbf{x}) \rangle + \langle \psi^{(0,2)}(\mathbf{x}) \rangle + \langle \psi^{(2,0)}(\mathbf{x}) \rangle + \langle \psi^{(2,2)}(\mathbf{x}) \rangle \end{aligned} \quad (44)$$

and the corresponding mean flux vector by

$$\begin{aligned} & \langle q^{[2,2]}(\mathbf{x}) \rangle \\ &= \langle q^{(0,0)}(\mathbf{x}) \rangle + \langle q^{(0,2)}(\mathbf{x}) \rangle + \langle q^{(2,0)}(\mathbf{x}) \rangle + \langle q^{(2,2)}(\mathbf{x}) \rangle \end{aligned} \quad (45)$$

## 7 EXAMPLE

Consider a rectangular grid of 20 x 40 square elements in the vertical plane (Fig. 1) having a width  $L_1 = 4\lambda$ , height  $L_2 = 8\lambda$ , and elements with sides  $0.2\lambda$ , where  $\lambda$  is the autocorrelation scale of  $Y$ . A water table boundary condition is imposed on the bottom of the domain. A constant deterministic flux  $Q = 0.5$  (all terms are given in arbitrary consistent units) is prescribed at the top boundary and zero pressure head at the bottom. The side boundaries are impermeable. A point source of magnitude  $QS = 1$  is placed inside the domain to render the mean flow locally divergent. The saturated hydraulic conductivity field is statistically nonhomogeneous through conditioning at three points, two above and one below the source.

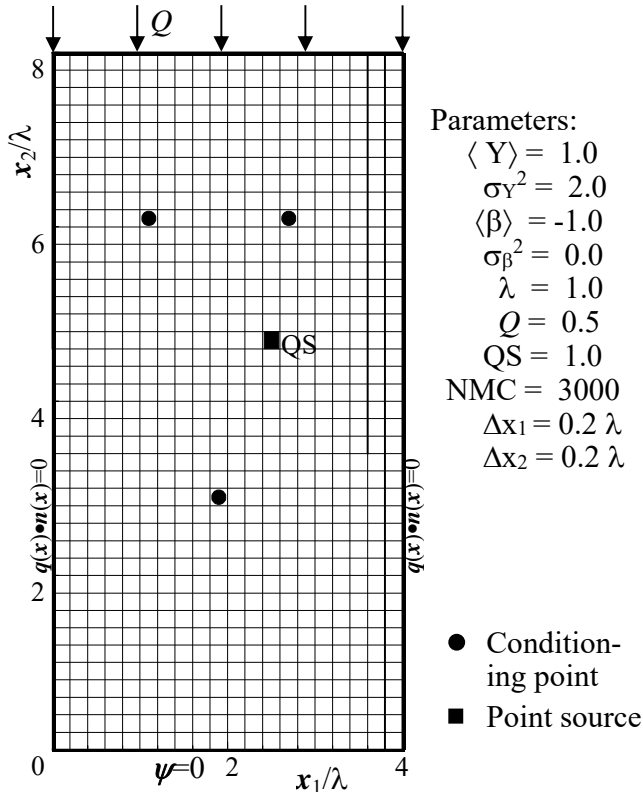


Figure 1. Problem definition and associated grid.

Our moment equations are free of any distributional assumptions. To solve the original stochastic flow equations by Monte Carlo simulation on the same grid (using standard finite elements), we assume that  $Y$  is multivariate Gaussian. Prior to conditioning,  $Y$  is statistically homogeneous and isotropic with exponential autocovariance

$$C_Y(\xi) = \sigma_Y^2 e^{-\xi/\lambda} \quad (46)$$

where  $\xi$  is separation distance,  $\sigma_Y^2$  is the variance of  $Y$ , and  $\lambda$  is its autocorrelation scale. We started by generating an unconditional random  $Y$  field on the grid by using a Gaussian sequential simulator, GCOSIM (Gómez-Hernández 1991), with  $\langle Y \rangle = 1$ ,  $\sigma_Y^2 = 2$  and  $\lambda = 1$ . We took its values at the conditioning points to represent exact "measurements" and generated NMC = 3,000 realizations of a corresponding nonhomogeneous  $Y$  field by the same method. We solved (1) - (4) for each realization with a constant  $\alpha$  by standard finite elements, and calculated sample mean pressure head and flux at each node, as well as sample variance and covariance of head and flux across the grid. This completed our conditional Monte Carlo simulation of flow in the example.

To render our direct solution of the conditional moment equations consistent with the Monte Carlo solution, we based it on the same conditional mean and autocovariance of  $Y$  as generated earlier by GCOSIM (in practical applications of our solution method, one would normally infer them geostatistically from measurements). Figures 2 - 7 compare various moments as obtained by these two methods of solution. Each of these figures includes a contour map and a vertical profile along the center line of the grid (at  $x_1/\lambda = 2.0$ ). Whereas the second order (in  $\sigma_Y$ ) mean pressure head virtually coincides with Monte Carlo (MCS) results (Fig. 2), the zero-order solution deviates from them slightly, especially near the upper flux boundary. Second-order horizontal (Fig. 3) and vertical (Fig. 4) mean fluxes correspond closely to their MCS counterparts, except for slight discrepancies near conditioning points and the point source. The zero-order results are also reasonably good, but somewhat less so.

It is not possible to obtain zero-order values of variance and covariance. Figure 5 shows a noticeable difference between contours of pressure head obtained directly to second order and by MCs. These differences are much smaller when viewed in profile. Variances of horizontal (Fig. 6) and vertical (Fig. 7) flux show very good agreement with MCS results, with some exceptions near conditioning points and the point source. Considering that our example concerns a strongly heterogeneous medium with  $\sigma_Y^2 = 2$ , our direct second-order finite element algorithm for solving the moment equations appears to work very well.

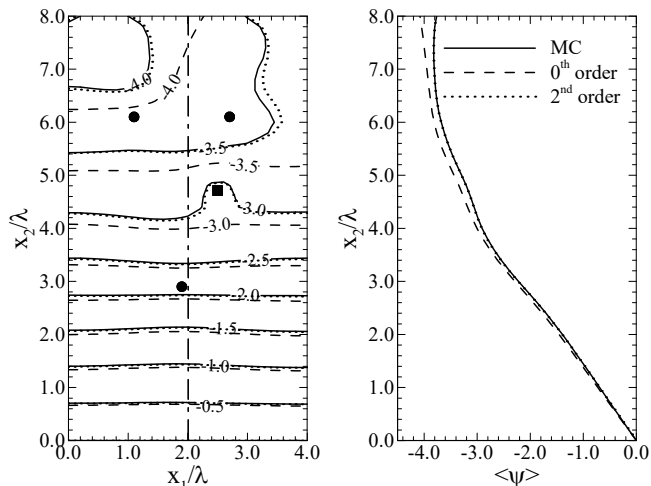


Figure 2. Contour map of mean pressure head and a vertical profile along  $x_1/\lambda=2.0$ .

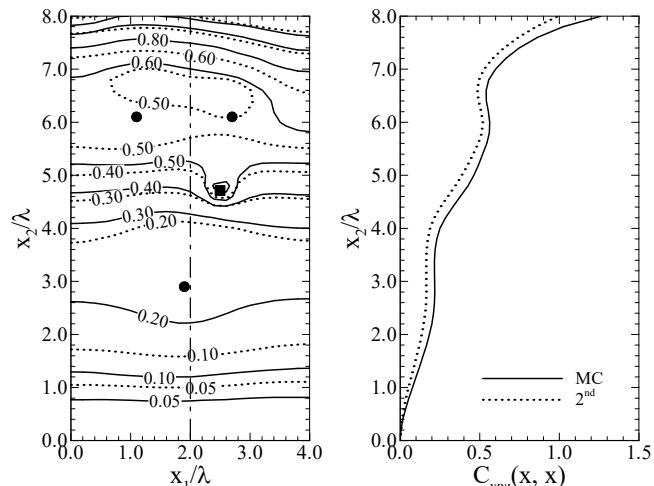


Figure 5. Contour map and vertical profile along  $x_1/\lambda=2.0$  of variance of pressure head.

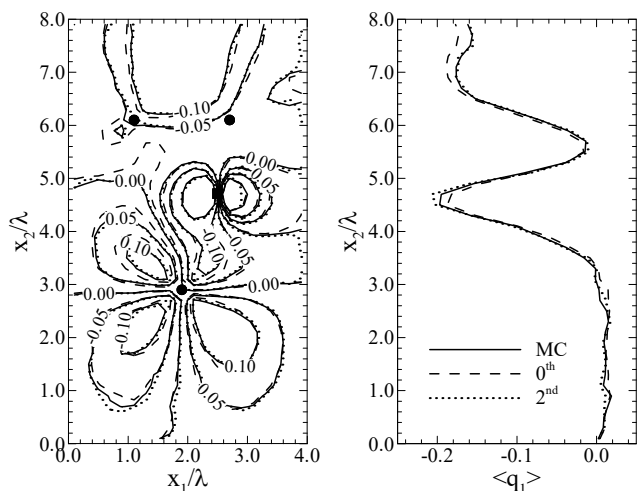


Figure 3. Contour map and vertical profile along  $x_1/\lambda=2.0$  of horizontal mean flux  $\langle q_1 \rangle$ .

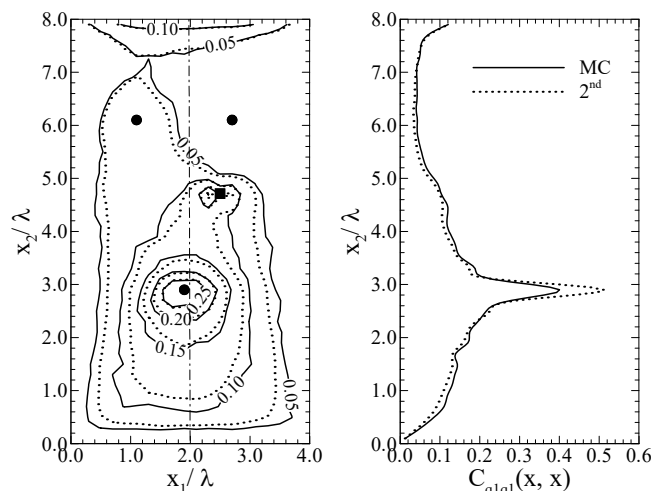


Figure 6. Contour map and vertical profile along  $x_1/\lambda=2.0$  of variance of horizontal flux.

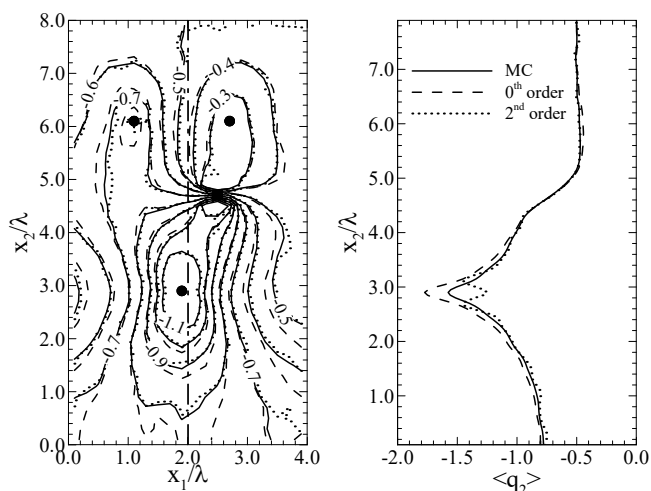


Figure 4. Contour map and vertical profile along  $x_1/\lambda=2.0$  of horizontal mean flux  $\langle q_2 \rangle$ .

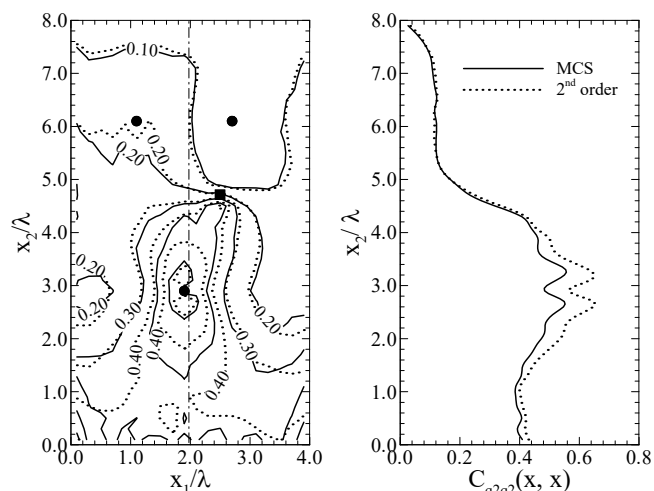


Figure 7. Contour map and vertical profile along  $x_1/\lambda=2.0$  of variance of vertical flux.

## 8 CONCLUSION

It is possible to linearize the steady state stochastic unsaturated flow equations by means of the Kirchhoff transformation, integrate them in probability space, and obtain exact integro-differential equations for the conditional mean and variance-covariance of transformed pressure head and flux. Approximating the latter equations to second order and solving them by finite elements for conditional mean pressure head, flux, and associated variance-covariance leads to results that compare favorably with those obtained by conditional Monte Carlo simulation, even under divergent flow in a soil that is strongly heterogeneous.

## 9 ACKNOWLEDGEMENTS

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