Mecánica Computacional, Volumen XIX, pp. 471-476
Compilado por: F. Quintana y S. Felicelli
San Carlos de Bariloche, Noviembre de 2000

A MONTE CARLO SIMULATION OF WATER FLOW IN VARIABLY SATURATED POROUS MEDIA

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RESUMEN

Se utiliza un método de simulación Monte Carlo para estudiar el flujo de aguas subterráneas en medios porosos fractales total o parcialmente saturados. El movimiento del agua se describe mediante la ecuación de Richards que se resuelve utilizando un procedimiento mixto híbrido de elementos finitos. Se considera que las heterogeneidades espaciales de los parámetros hidráulicos obedecen a la estadística de un movimiento fraccional Browniano (fBm) o de un ruido fraccional Gaussiano (fGn). Se presenta un ejemplo numérico para ilustrar la implementación del algoritmo y el cálculo de los momentos estadísticos de las principales variables.

ABSTRACT

A Monte Carlo simulation method is employed to study groundwater flow in variably saturated fractal porous media. The water movement is assumed to be described by Richards' equation which is solved using a hybridized mixed finite element procedure. Spatial heterogeneties in the hydraulic properties are assumed to obey fractional Brownian motion (fBm) or fractional Gaussian noise (fGn) statistics. A numerical example showing the implementation of the algorithm including the calculation of the statistical moments of the main variables is presented.

INTRODUCTION

Field studies in soils sciences and hydrology during the last two decades have demonstrated extensive variability in saturated and unsaturated hydraulic conductivities and water retention properties. This conclusion has led to the development of stochastic models for the basic understanding and the prediction of water flow and contaminant transport processes in geological environments.

To describe variably saturated flow and transport, the constitutive relationships of hydraulic conductivity (K) versus pressure head (h) and water content (θ) versus h must be specified. At field scale, these constitutive relationships exhibit a high degree of spatial variability [1] and they are regarded as stochastic functions. As a consequence the flow equations have to be treated in a stochastical framework.

The Gardner-Russo model [2,3] is commonly used to describe functional relationships in most stochastic flow analyses. The main parameters of this model are the saturated conductivity K_s and the soil pore size distribution α.

The spatial variability of K_s has been widely studied and it is commonly accepted that K_s follows approximately lognormal distributions. Recently, the concept of fractal geometry has been used to describe continuously evolving scales of heterogeneity. Neuman [4], Kemblowski and Chang [5] and Molz and Boman [6] had reported evidences of fractal structure in K_s distributions in different soils. They found that K_s distributions can be described by related stochastic functions known as fractional Gaussian noise (fGn) and fractional Brownian motion (fBm). The concepts of fBm and fGn are generalizations of the classical concepts of Gaussian noise and Brownian motion.

The experimental information on spatial distribution of α is very limited. Russo and Bouton [1] found that α has also a lognormal distribution and negligible correlation with K_s.

In this paper we use the Monte Carlo simulation method in conjunction with a fBm and fGn field generator to analyze the water flow in a stochastic farmework. In each realization the Richards' equation is solved using a hybridized mixed finite element procedure.

GENERATION OF fBm AND fGn

In this section we present a brief description of the spectral method used for the synthetic generation of fBm and fGn. We consider a stochastic function which has the form $\log F(\mathbf{x}) = \langle \log F \rangle + f(\mathbf{x})$ where $\langle \log F \rangle$ is a constant mean and $f(\mathbf{x})$ is a perturbation field which obey fBm or fGn statistics.

The spectral density of a fBm/fGn has the form of a power law:

$$S_{ff}(\mathbf{k}) = \frac{S_o}{|\mathbf{k}|^\beta} \quad (1)$$

where S_0 is a normalization constant, $\mathbf{k}$ is the spatial frequency (wave number), and β is a parameter related to the Hurst coefficient H and the Euclidian dimension E given by

$$\beta = \begin{cases} 2H + E & \text{for a fBm} \\ 2H + E - 2 & \text{for a fGn.} \end{cases} \quad (2)$$

It should be noted that in the case of a fGn realization the spectral density given by (1) and (2) is only an approximate expression because it is associated with an approximation to the autocovariance function; a closed-form expression of the accurate spectral density is not available. On the other hand, the spectral density of a fBm process is associated with the corresponding variogram [7].

The value of the Hurst exponent H indicates the type of correlation and degree of persistence in fGn and fBn distributions. The range of H which is interesting and physically meaningful is $0 < H < 1$ [7]. For $H > 0.5$ there is a positive and infinite correlation both for fGn and the increments of fBm while for $H < 0.5$ this correlation is negative and infinite. When H approaches 0.5 the correlation becomes essentially zero and in this special case the classical Gaussian noise and Brownian motion are obtained. The Hurst coefficient H is related to the fractal dimension D by the equation $H = 1 + E - D$ [9]. It is important to remark that the values of H can be determinated from measured data and it is also possible to discrimine fBm from fGn distributions [8].

The spectral density $S_{ff}(\mathbf{k})$ has a singular point at zero spatial frequency which corresponds to the case of an infinitely large porous media. However, the limit of the heterogeneity could not be larger than the aquifer size. Therefore there is a lower frequency cutoff $\mathbf{k}_{min}$ which is determinated by the lengh of the domain. We also consider an upper frequency cutoff $\mathbf{k}_{max}$ proportional to the inverse of the finite element mesh used for the numerical simulation of water flow.

In order to obtain an expression of S_0 in term of the variance σ_f^2 we integrate the spectral density (1) over the frequency domain in the range $(\mathbf{k}_{min}, \mathbf{k}_{max})$. Then the spectral density of a fBm and a fGn can be expressed as follows:

$$S_{ff}(\mathbf{k}) = \begin{cases} C(E)\sigma_f^2(E-\beta)\left[2[k_{max}^{E-\beta} - k_{min}^{E-\beta}]k^{\beta}\right]^{-1} & k_{max} < |\mathbf{k}| < k_{min} \\ 0 & \text{elsewhere} \end{cases} \quad (4)$$

where $C(E) = 1, \pi^{-1}, (2\pi)^{-1}$, for $E = 1, 2, 3$, respectively.

To generate a fBm or a fGn realization we proceed here in the spirit of Voss [9]. The first step is to generate a set of uniformly distributed random numbers associated with the center of each cell of the finite element mesh using a random number generator. Then the fast Fourier transform (FFT) of this set of numbers is taken and the resulting numbers are multiplied by a transfer function $T(\mathbf{k})$ proportional to $[S_{ff}(\mathbf{k})]^{1/2}$ in the wave number space. Finally, taking the inverse FFT a set of numbers with the desired spectral density (4) is obtained.

The Constitutive Relations for the Flow Model

The Gardner Russo model was used to describe retention and hydraulic conductivity curves [2,3]. This model reads as

$$K(\mathbf{x}, h) = K_s(\mathbf{x})\exp\big(\alpha(\mathbf{x})h\big) \quad (5)$$

$$\theta(\mathbf{x}, h) = \big(\theta_s(\mathbf{x}) - \theta_r(\mathbf{x})\big)\Big(\exp\big(0.5\alpha(\mathbf{x})h\big)\big(1 - 0.5\alpha(\mathbf{x})h\big)\Big)^{2/(m(\mathbf{x})+2)} + \theta_r(\mathbf{x})$$

where θ_r and θ_s are the residual and saturated water content, respectively, and m is a parameter related to tortuosity.

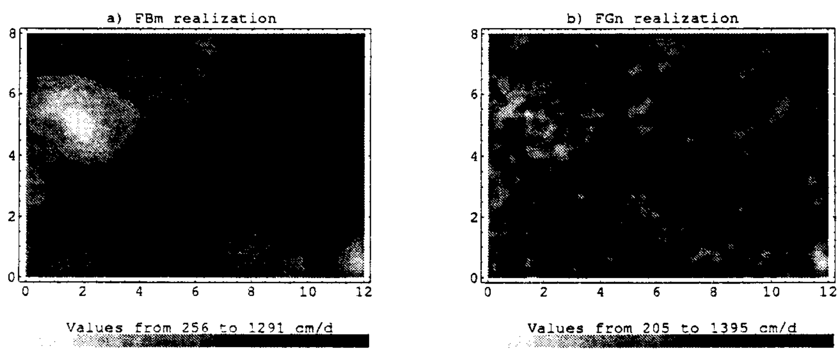

Figure 1: Realization of K_s field generated from fBm and fGn distibutions.

For simplicity we let $m = 0$ in this study. The variabilities of θ_r and θ_s are likely to be small so that we consider them constants over the domain. Then, the local heterogeneities are modelled assuming that both K_s and α are stochastic processes obeing either fBm or fGn statistics.

Table I gives the values chosen to generate the realizations and Figure 1 shows 2D realizations of the conductivity field K_s generated as fBm and fGn processes.

	K_s (cm/s)	α (cm^{-1})
$< F >$	0.0058	0.028
σ_f^2	0.1	0.010

H	0.8
θ_s	0.6
θ_r	0.1

Table I: Parameters of the Gardner Russo model.

NUMERICAL SOLUTION OF THE FLOW EQUATION

We will consider the numerical simulation of water flow in a rectangular domain Ω. It will be assumed that water flow obeys Richards' equation stated in the form

$$\begin{aligned} &i) \quad \frac{\partial \theta(h)}{\partial t} + \nabla \cdot \mathbf{q} = 0 \\ &ii) \quad \mathbf{q} = -K(h)\nabla(h+z) \end{aligned} \tag{6}$$

where $\mathbf{q}$ is the water flow, z denotes the soil depth assumed to be positive upward, and t is time. The corresponding boundary conditions were chosen to be of Dirichlet type on the left and right boundaries and of Neumann type on the bottom and top boundaries. The initial condition was selected as that of hydrostatic equilibrium.

Equation (6) was solved employing a hybridized mixed finite element procedure in space combined with a backward Euler in time scheme and a Picard iteration with adaptive time step as explained in [10]. This procedure produces perfectly mass conservative numerical solutions and accurately aproximations of both pressure head and water flow.

The Monte Carlo simulation method consists in solving Richards' equation for a large number of realization of K_s and α. The simulation is terminated after the mean field of a particular variable (θ, for example) have converged to within a small tolerance. This tolerances is taken to be 1% of the mean field.

NUMERICAL EXAMPLE

In order to show the implementation of the algorithm we will consider the effect of infiltration in a rectangular domain having a width of 1200 cm and a depth of 800 cm, with a horizontal water table situated at 650 cm from the top bondary. The hydraulic properties of the porous media are described by the parameters shown in Table I.

The selected boundary conditions are a constant infiltration of 1.5 cm/day applied in a centered interval of 400 cm at the top boundary, no-flow at the bottom boundary and specified pressure heads corresponding to the hydrostatic state at the two lateral sides.

Figure 2 shows the water content after 25 days of simulation for a realization of fBm and fGn distributions. In both simulations the effect of the local heterogeneities is clearly observed.

To insure the convergence of the mean fields of all the variables we runned 200 realizations. The average values and variances for the water content, pressure head and z-component of water flow are shown in figures 3, 4 and 5, respectively.

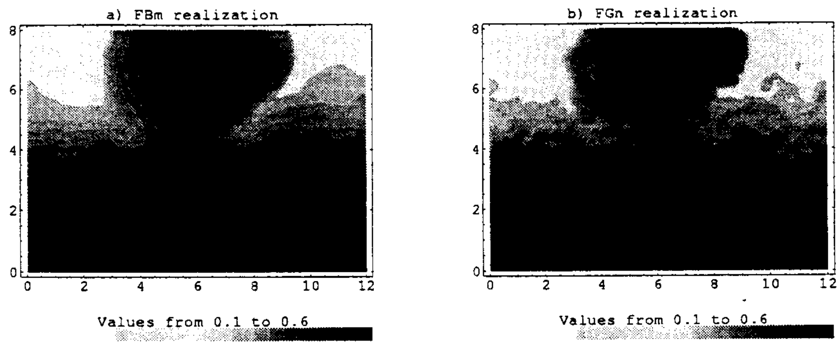

Figure 2: Water content realizations for fBm and fGn distributions.

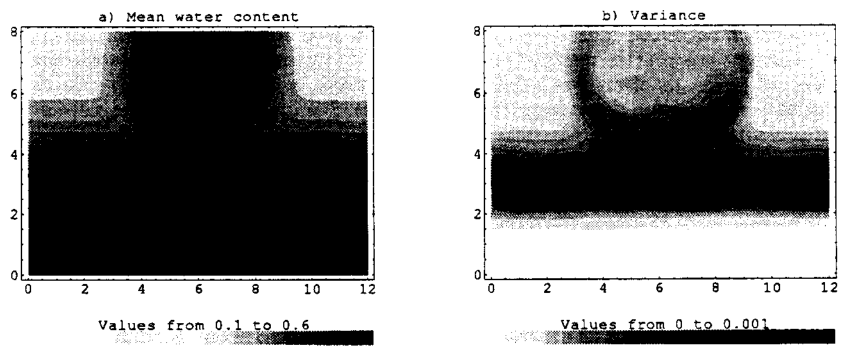

Figure 3: Mean water content and variance for a fBm distibution.

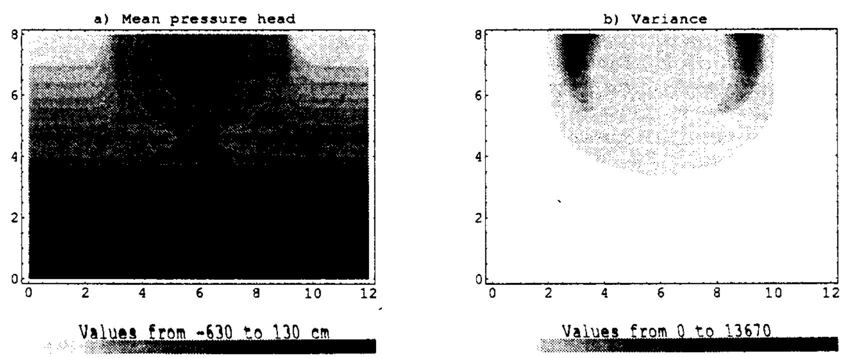

Figure 4: Mean pressure head and variance for a fBm distibution.

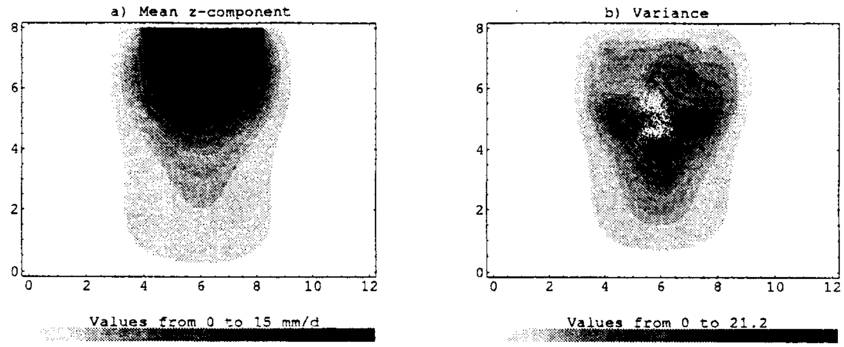

Figure 5: Mean z-component of water flow and variance for a fBm distibution.

CONCLUSIONS

We have presented a numerical method to include the effect of local heterogeneities in the hidrogeological variables employing the theory of stochastic processes and relating filed measurements with the spectral properties of such variables. The method employes a robust and mass conservative finite element procedure to compute accuratly the water flow in this type of heterogeneous soils. This procedure can be combined with the solution of the transport equations to obtain concentration statistics of contaminant substances in soils.

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