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Random walk path solution to groundwater flow dynamics in highly heterogeneous aquifers

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ABSTRACT

Random walk path methods including walk on spheres and walk on rectangles have been used to solve elliptic and parabolic partial differential equations (PDEs). These methods are able to provide not only the pointwise solutions to the linear PDEs but also contributions of boundaries and all source/sink terms as an analytical solution does. However, due to difficulty in dealing with heterogeneity, these methods cannot be applied to groundwater flow problems in highly heterogeneous aquifers. A novel method called walk on grid (WOG) is proposed based on lattice random walk to overcome the difficulty. WOG algorithm is verified in a 1D homogeneous transient problem, a 1D heterogeneous steady-state problem, a 2D heterogeneous transient problem and a 3D optimization problem. It is demonstrated that WOG is effective in solving groundwater flow problems in highly heterogeneous confined aquifers. Probabilities of walkers arriving at prescribed boundaries (terminal weights) and source counts may be useful for characterization of medium heterogeneity. WOG method sheds a new light on solving the PDEs of complicated groundwater problems in a changing environment and on analyzing medium heterogeneity.

1. Introduction

In groundwater modelling, researchers generally use a set of governing equations to describe physical processes like water flow, solute or heat transport and so on. Most if not all of these governing equations are PDEs of diffusion type, which often have to be solved through analytical or numerical approaches. Analytical solutions are able to provide comprehensive information of variables in the spatial/temporal domain under study including contributions from each component in the model. Unfortunately, analytical methods strongly rely on models' simplification (often oversimplification) of reality and substantially impose remarkable restrictions on range of application. When analytical solutions are unavailable, hydrogeologists resort to numerical methods e.g. finite difference (FDM) and finite element methods (FEM) for approximate solutions. Traditional numerical methods solve the governing equations for values of variables which hardly allow one to explicitly check the contributions of model components (source terms, boundary or initial conditions) in those values without assistance of additional tools e.g. sensitivity analysis.

Random walk path method is a PDE-solving method that solves elliptic and parabolic PDEs via random walk simulation. Based on Feynman-Kac formula, it expresses the pointwise solutions in form of linear combinations of prescribed conditions and source/sink terms.

It is noteworthy to distinguish this method with particle tracking method. Though based on random walk (Brownian motion) as well, the widely-documented particle tracking method (LaBolle et al., 1996; Valocchi and Malmstead, 1992; Ramirez et al., 2008; among many others) is substantially different from the random walk path method on mathematical bases. The particle tracking method is sometimes known as random-walk particle method or random walk method. To avoid confusion, we refer to it as particle tracking method and the method demonstrated in this paper is termed random walk path (RWP) method. The particle tracking relies on similarity between advection-diffusion equation and Fokker–Planck equation (LaBolle et al., 1996), or more precisely Smoluchowski equation (Risken, 1984). It is based on "snapshotting" of a large number of particles and known as one of Lagrangian methods to solve solute transport problems. Fokker-Planck equation is also known as Kolmogorov forward equation (KFE), which describes time evolution of probability density after time t, given that probability density at time t is known. In contrast, Kolmogorov backward equation (KBE), the adjoint of KFE, traces back the historical probability density before time t under the condition of an occurrence at location $\mathbf{x}$ and time t. KBE directly results in Feynman-Kac theorem and RWP method is an application of the theorem. Interested readers are referred to literature on stochastic differential equations, e.g. Kallianpur and Sundar (2014) for rigorous formulations and proofs behind KBE and KFE.

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Below it will be shown that RWP method relies on trackback of many random paths linking a single point with prescribed boundaries. Feynman-Kac theorem and implementation of RWP will be explained below in context of groundwater flow simulation.

First scheme of RWP method (random walk on spheres, WOS) was proposed by Muller (1956) to solve the Laplace equation with Dirichlet boundaries. Muller's method is efficient for elliptic (steady-state) equations but not for parabolic equations due to difficulty in simulating the first exit time (i.e. the moment the walker stops at terminals). Later, walk on rectangles (WOR) was used to overcome this difficulty (Milstein and Tretyakov, 1999) but preferably applicable to problems with boundaries of polygonal shape (Deaconu and Lejay, 2006). Some applied WOS and WOR to simulate pressure in dual-porosity media (Campillo and Lejay, 2002), evaluating some physical properties of large molecules such as reaction rates and electrostatic energy (Mascagni and Simonov, 2004), estimate effective permeability based on pore geometry (Simonov and Mascagni, 2004) and so on. Both WOS and WOR work in the grid-free spatial domain but time is discretized to steps. That is, a temporally stepwise random walk occurs in a spatially continuous domain. Since the walk path is not subject to predetermined discrete grid, in theory the walker may make a huge step in a single move and exit the domain quickly. It allows the walker completing a walk path fast and reduces computational cost in homogeneous media. In heterogeneous media, it is much harder to simulate random walks. Bhattacharya and Gupta (1984) studied simulation of random walk in a cylinder with smoothly-varying properties, the result of which is quite limited to simple problems. As to a single interface of discontinuity, some models such as skew Brownian motion (Itô and McKean, 1963, 1974; Etore, 2006; Ramirez et al., 2008) can be used to handle layered media. If the medium shows heterogeneity of irregular shape, the walker has to be replaced to a new position according to medium heterogeneity every time the walker passes an interface of parameter discontinuity (Lejay and Martinez, 2006; Lejay and Marie, 2013; Lejay and Pichot, 2012). Some studies attempted to apply WOS in bi-material problems (Lejay and Pichot, 2016; Maire and Nguyen, 2016). When the medium is highly heterogeneous, the interface passage may occur in uncertain high frequency and the aforementioned replacement is extremely hard and impractical. Besides, how to handle various boundary conditions (including pure Neumann, mixing, Robin boundaries) has recently been studied (Maire and Tanré, 2012; Maire and Nguyen, 2016). For these reasons, RWP method has not been tested or investigated in subsurface modelling which deals with complex components including high heterogeneity, various boundary conditions, time-variant sink/source terms in practical problems. In this study a novel RWP scheme called walk on grids (WOG) based on lattice random walk is proposed. The objectives of this study include summarizing the theoretical background of RWP methods and ways of dealing with various boundary conditions, introducing the implementation of WOG method in groundwater modelling context, and preliminarily demonstrating the capability of WOG solution in groundwater modelling and management.

The rest of this paper is organized as follows. In Section 2, the theory and implementation of RWP method are introduced. In Section 3, we conduct a series of experiments (one-/two-/three-dimensional, homogeneous/heterogeneous, steady-state/transient problems) to explore the capability of WOG. The experimental results are discussed in Section 4 and conclusions are drawn in Section 5.

2. Methodology

2.1. Formulation of the problem

The basic governing equation for transient groundwater flow in confined and isotropic aquifers is

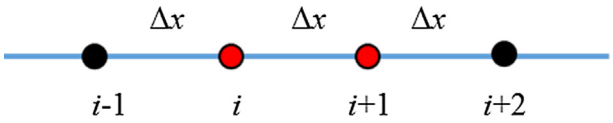

Fig. 1. A uniform grid. Knowns and unknowns are denoted by black and red dots, respectively. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

$$\begin{cases} \nabla\cdot(K(\mathbf{x})\nabla h(\mathbf{x},t)) + w(\mathbf{x},t) = S_s\frac{\partial}{\partial t}h(\mathbf{x},t), x \in D \\ h(\mathbf{x},0) = H_0(\mathbf{x}) \\ h(\mathbf{x},t) = H_D(\mathbf{x},t), x \in \Gamma_D \\ K(\mathbf{x})\frac{\partial}{\partial n}h(\mathbf{x},t) = -q(\mathbf{x},t), x \in \Gamma_N \end{cases} \tag{1}$$

where $\mathbf{x}$ is a spatial vector. $K(\mathbf{x})$ is the location-dependent hydraulic conductivity. $w(\mathbf{x},t)$ is the source/sink term. S_s is specific storage. D is the aquifer domain. Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively. n is the outward length normal to the boundary Γ_N. We would like to solve this equation via Monte Carlo method in the domain D. What we are interested in is not only the certain value of $h(\mathbf{x},t)$ but also the explicit contribution of $H_0(\mathbf{x})$, $H_D(\mathbf{x},t)$, $q(\mathbf{x},t)$ and $w(\mathbf{x},t)$ in $h(\mathbf{x},t)$.

2.2. Theoretic basis of RWP method

2.2.1. The link between PDEs and random walk

Consider a simple 1D Laplace equation: $\Delta u = 0$. Assume that the values at points $i-1$ and $i+2$ (u_{i-1} and u_{i+2}) are already known and that one wants to solve the equation at point i on a uniform grid (see Fig. 1 below). Intuitively, one can express the approximate solution u_i in terms of u_{i-1} and u_{i+2}. According to the original equation, one has an approximation (second-order central difference) $(u_{i-1} + u_{i+1} - 2u_i) \approx 0$ and $(u_i + u_{i+2} - 2u_{i+1}) \approx 0$, that is,

$$\begin{cases} u_i \approx \frac{1}{2}u_{i-1} + \frac{1}{2}u_{i+1} \\ u_{i+1} \approx \frac{1}{2}u_i + \frac{1}{2}u_{i+2} \end{cases} \tag{2}$$

And one can easily solve the equation set to obtain

$$u_i \approx \frac{2}{3}u_{i-1} + \frac{1}{3}u_{i+2}. \tag{3}$$

Or in more general form,

$$u_i = \sum_{k=1}^{N_T} r_k u_k^{(T)} \tag{4}$$

where $u_k^{(T)}$ denotes known values (at prescribed boundaries); the subscript (T) stands for "terminal", which terminates the chains of unknowns by known values; here $u_1^{(T)} = u_{i-1}$, $u_2^{(T)} = u_{i+2}$, $r_1 = \frac{2}{3}$, $r_2 = \frac{1}{3}$.

Eqs. (2)-(4) can be understood in perspective of probability (though it seems totally irrelevant to any randomness). Assume U_i to be a random variable at point i, and that the probability of $U_i = U_{i-1}$ is $p_- = \frac{1}{2}$ and the probability of $U_i = U_{i+1}$ is $p_+ = \frac{1}{2}$; similar for point $i+1$. We can define a random walk on a domain shown in Fig. 1 based on these probabilities: at points i or $i+1$, a walker can move to left or right with probability p_- and p_+, respectively; and the walker will continue moving based on "either-or" operation until it reaches point $i-1$ or $i+2$ (i.e. it arrives at any terminal and exits the domain). The walkers stops because the random variable equals a known value instead of another random variable, i.e. $U_i = u_{i-1}$ at point $i-1$ and $U_i = u_{i+2}$ at point $i+2$. It can be easily shown by statistics that the walker stops at point $i-1$ with probability $\frac{2}{3}$ (i.e. "exit probability" or "hitting probability" r_1) and stops at point $i+2$ with probability $\frac{1}{3}$ (i.e. "exit probability" r_2). In the sense of probability, $u_i = \langle U_i \rangle = \frac{2}{3}u_{i-1} + \frac{1}{3}u_{i+2}$, which is exactly Eq. (3). $\langle\ \rangle$ denotes expectation. The coefficient r_k represents the (conditional) probability