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Abstract. A continuous-time random-walk method is introduced for applications to transport processes in random media. The method is efficient and is easily parallelizable. It can be used to calculate the diffusivity of homogeneous mixtures of many components, with applications to effective permeability and conductivity measurements. It is also applicable to diffusion-limited aggregation in random media and to determining connected regions of high permeability in geological models of petroleum reservoirs.

1. Introduction

In two previous papers [14, 16], a random-walk method was introduced for calculating the effective permeability of a homogeneous mixture of many-permeability components distributed on a large, three-dimensional grid. The method involved extracting the diffusivity from the time-evolution of the mean-square displacement of a cloud of random walkers moving through the system, and determining the permeability via an Einstein relation. It was an extension of the 'blind ant' algorithm used to calculate the conductivity of conductor–insulator systems in percolation theory and porous-media problems [20, 23]. In its previous formulation, the random-walk algorithm could efficiently be applied to homogeneous mixtures of two components (i.e. sand–shale sytems) [14, 16] or of many, uniformly distributed components (i.e. patchwork systems) [15]. However, it became inefficient when applied to arbitrarily (e.g. lognormally) distributed permeability components. This is because the probability for a walker to move from one site to its neighbour was given by the harmonic mean of the adjacent site permeabilities, all normalized to lie between zero and one. When the permeability components were distributed continuously with a large variance, the walkers moved inefficiently through the system, often waiting at the same site for many simulation steps.

In this paper it will be described how the concept of continuous-time random walks can be used to define an algorithm in which the walkers make a move at every simulation step, with the time being updated from a first-passage time distribution. The algorithm is efficient and can be applied to lognormal permeability distributions by using appropriate time scaling. Once again, the main focus of the paper is on calculating the effective permeability of large, three-dimensional systems of gridblocks for application to petroleum reservoir simulators. However, some discussion will also be given to applications of the method to calculating effective conductivities of continuum systems and performing diffusion-limited aggregation in random media.

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2. Upscaling permeability for reservoir simulators

The reservoir simulators used to predict fluid flow in petroleum reservoirs are based on finite-difference methods. The reservoir is modelled by a system of homogeneous gridblocks to which 'effective' property values (e.g. effective permeability) are assigned. The problem of determining the appropriate effective values, which correctly model the effects of heterogeneities on scales smaller than the gridblock scale, has been the subject of much recent research in the petroleum industry [2–5, 11, 12]. If some idea of the distribution of permeability inside the gridblock can be gained, e.g. from well logs and/or cores, then Monte Carlo simulations can be performed to calculate the effective permeability at the scale desired for reservoir simulations [4]. This is a tedious, but accurate approach. When insufficient data are available, or when a rough approximation of the effective permeability is considered to be acceptable, fast analytical methods can be used (NB a review of analytical methods is given in McCarthy [16]).

An alternative approach, combining the advantages of speed and accuracy, is to perform Monte Carlo simulations for a variety of commonly occurring permeability distributions and to parameterize the results by fitting them to a characteristic functional form. Then, effective permeabilities can be found by a table look-up. This is a similar approach to that used for estimating the conductivities of rocks. In that case, the characteristic functional form is derived from Archie's law [10].

In a previous study [16], the effective permeability of sandstone–shale distributions was parameterized using a power-averaging law, categorizing the distributions in terms of their anisotropy and correlation length. It was necessary to perform simulations on large, three-dimensional systems of gridblocks (i.e. 100^3) because accurate calculations of the effective permeability can only be made when the gridblock scale is much smaller than (and the system scale much larger than) the scale of correlations. For that reason, a random walk method was used rather than the traditional method of solving the flow equations using finite differences. Random walk methods are more efficient for large systems [23].

Sandstone–shale distributions, in which the permeabilities of the two components differ by orders of magnitude, are an important practical case. Another practical case, often found in analyses of rock samples [4], is that of lognormally distributed permeability components. An efficient random-walk algorithm for this case is described in section 3. It will enable extensive Monte Carlo simulations to be performed in the future.

3. Random-walk methods

Darcy's law for the flow of a single-phase fluid in a porous medium gives

$$q = -(k/\mu)\nabla p \tag{1}$$

where q is the volumetric flow rate per unit area, k is the permeability, μ is the viscosity and p is the pressure. The quantity $k/\mu = \kappa$ is known as the mobility, and is effectively equivalent to the permeability in the context of this paper.

Assuming incompressible flow, i.e. $\nabla \cdot q = 0$, leads to the following equation for the pressure:

$$\nabla \cdot (\kappa \nabla p) = 0\,. \tag{2}$$

To compute the effective permeability, K_x, for flow in the x-direction through a cubic system of gridblocks with permeabilities κ_i, the usual procedure is to solve the pressure

equation using a finite-difference scheme with constant pressure boundaries on the x-faces of the cube and no-flow boundaries on the y- and z-faces of the cube. The integrated flux over any y–z cross-section of the cube is equated with the flux corresponding to flow through a cube of uniform permeability K_x. Similar computations must be performed for flow in the y and z directions in order to find K_y and K_z. To compute the value of the effective permeability which is characteristic for a particular distribution, an ensemble average is taken over the results obtained for several realizations of the permeability field κ_i.

When using a random-walk method, the value of the permeability in different directions can be found in one simulation by monitoring the mean square displacement in different directions separately. The boundary conditions correspond to the pressure tending to zero at infinity.

In order to devise a random-walk algorithm for calculating effective permeability, it is necessary to construct a random-walk process in the gridblock system which yields a steady state diffusion equation identical in form to (2). In a homogeneous system of permeability K this is straightforward—at each simulation step, a walker moves to any of its neighbouring sites with equal probability. In the continuum limit, the time-evolution of a cloud of such random walkers, starting from an arbitrarily chosen site in the system, is governed by the diffusion equation

$$\frac{\partial u}{\partial t} = D\nabla^2 u \tag{3}$$

where $u(x, t)$ is the probability density of walkers at point x at time t, and D is the diffusivity. In the steady state, this is identical in form to (2). A direct correspondence can be made between $\lim_{t\to\infty} u(x, t)$ and $p(x)$, and between D and K.

To calculate the diffusivity of the system it is not necessary to let the random-walk process reach its steady state (i.e. it is not necessary to *solve* the flow equations). Rather, diffusivity can be found from the characteristic random walk relation

$$\langle R^2(t)\rangle \sim 6Dt \tag{4}$$

where $\langle R^2(t)\rangle$ is the mean square displacement of the cloud of random walkers at time t. Using Einstein's relation, a direct correspondence can then be made between diffusivity and permeability (or conductivity, in the case where one is considering conductive components). This technique is what makes the random-walk method an efficient alternative to finite differences. The question of efficiency will be addressed in the section on numerical simulations (i.e. section 5).

For two-component systems in which one component is permeable and the other impermeable, a random walk process called the 'blind ant' can be used. At each simulation step, a walker chooses one of its neighbouring sites at random. If the chosen site is permeable, the walker moves there, otherwise it stays put. In either case, the time is incremented by one unit. The blind ant algorithm has been used extensively in calculations of the diffusivity and critical exponents of diffusive processes on percolation clusters [7, 8, 22]. It has also been used in studies of electrical transport in homogeneous disordered continuum systems [20, 23].

Let us consider a random-walk process in a heterogeneous system in one dimension. The discrete diffusion equation for the walk process is

$$u(i, t+1) = u(i+1, t)b_{i,i+1} + u(i-1, t)b_{i-1,i} + u(i, t)[1 - b_{i,i+1} - b_{i-1,i}] \tag{5}$$

where $b_{i,j}$ is the probability for a walker to move from site i to its neighbouring site j. Rearranging gives

$$u(i,t+1)-u(i,t)=[u(i+1,t)-u(i,t)]b_{i,i+1}-[u(i,t)-u(i-1,t)]b_{i-1,i} \tag{6}$$

which is a discretized form of

$$\frac{\partial u}{\partial t}=\frac{\partial}{\partial x}\left[b\frac{\partial u}{\partial x}\right]. \tag{7}$$

In three dimensions this becomes

$$\frac{\partial u}{\partial t}=\nabla\cdot(b\nabla u). \tag{8}$$

In order to make the correspondence with (2), it remains to appropriately choose the bond probabilities $b_{i,j}$ in terms of the site permeabilities κ_i. This must be done in such a way as to satisfy the boundary conditions for the continuum fluid flow equations at the interface between regions of different permeability, i.e.

(i) The normal component of flow rate per unit area is continuous across the boundary:

$$\boldsymbol{q}_i\cdot\boldsymbol{n}=\boldsymbol{q}_j\cdot\boldsymbol{n} \tag{9}$$

where $\boldsymbol{n}$ is normal to the boundary and $\boldsymbol{q}_i$ and $\boldsymbol{q}_j$ are measured just inside regions i and j respectively.

(ii) Pressure is continuous at the boundary:

$$p_i=p_j. \tag{10}$$

In discussions of finite-difference schemes (e.g. Aziz and Settari [1]) it is shown that the appropriate choice to make is the harmonic mean of the site permeabilities. For a random-walk process, these have to be normalized to lie between zero and $1/z$, where z is the coordination number of the lattice, so the choice becomes

$$b_{i,j}=\frac{1}{6B}\frac{2\kappa_i\kappa_j}{\kappa_i+\kappa_j} \tag{11}$$

where B is the maximum of the set of intersite harmonic means. Then, the generalized blind ant process for random walkers in a heterogeneous system becomes: at each simulation step, a walker chooses one of its neighbouring sites at random and moves there with probability $b_{i,j}$. The time is incremented by one unit.

4. Proposed CTRW method

The blind ant process described in section 3 has been used successfully to calculate effective permeabilities of homogeneous mixtures of two non-zero permeability components [14, 16] and of many, uniformly distributed permeability components [15]. However, as explained in the introduction, it is inefficient when applied to arbitrarily (e.g. lognormally) distributed permeability components.

According to the generalized blind ant rules, a walker can be trapped for many simulation steps at any site which is surrounded by low bond probabilities. A more efficient

Table 1. Results for uniform continuous distributions in the interval $[a, b]$. Comparison of finite differences (FD) with the CTRW algorithm for various maximum times.

	[0, 1]	[1, 9]	[1, 99]	[1, 9999]
Arithmetic mean	0.50	5.00	50.0	5000
Geometric mean	0.368	4.36	38.2	3680
K (FD)	0.377 ± 0.002	4.29 ± 0.01	38.5 ± 0.2	3790 ± 20
K (CTRW) 10^3 steps	0.377 ± 0.009	4.26 ± 0.11	38.0 ± 1.0	3810 ± 170
K (CTRW) 10^4 steps	0.378 ± 0.008	4.29 ± 0.11	38.2 ± 0.5	3760 ± 130

process would make the walkers move at every simulation step. A process of this type which has been used in the two-component, permeable/impermeable case is called the 'myopic ant'. The myopic ant only chooses from those of its neighbours which are permeable, and it always makes a move. However, in its usual implementation, the myopic ant process does not correspond to the appropriate diffusion process (equation (8)) and cannot be used to calculate diffusivities. Its use has been restricted to calculating critical exponents for diffusion on percolation clusters [8, 13, 18, 22] (NB the critical exponents are the same for the blind and myopic ants).

To define a generalized myopic ant process which has the correct time evolution, we have used the concept of continuous-time random walks (CTRW) [7]. In CTRW processes, the walker makes a move at every simulation step and the time is updated according to a first-passage time distribution. For a Poisson process such as that described by (5), the first-passage time distribution is exponential. So, the proposed process is as follows:

(i) Set the probability for a walker to stay at the same site to zero.

(ii) Normalize the probabilities to move to neighbouring sites according to

$$\bar{b}_{ij} = \frac{b_{ij}}{\sum_{i=1}^{z} b_{ij}}. \tag{12}$$

(iii) At each simulation step, a walker chooses one of its neighbouring sites with a probability weighted by $\bar{b}_{ij}$ and moves there.

(iv) The time is updated according to an exponential waiting-time distribution [19]

$$t_{n+1} = t_n - \frac{1}{\sum_{i=1}^{z} b_{ij}} \log(\text{rand}) \tag{13}$$

where rand is a uniform random number in the interval [0, 1].

5. Numerical simulations

In order to compute the time evolution of the mean square displacement of a cloud of random walkers moving according to the proposed rules, the following procedure is used. A maximum time is specified and each walk is discretized into time intervals of fixed length. For example, if the maximum time is set at 10^3 units, then one could use 10^2 time-bins of length 10. At each simulation step, a walker makes a move to a neighbouring site and the new value of the displacement is added to the time-bin corresponding to the discretized updated time. The old value of the displacement is added to all the time-bins between the old one and the new one. If the updated time is greater than the maximum time, the old value of the displacement is added to all the remaining time-bins and a new walk is started. Each walk is started from a randomly chosen site.

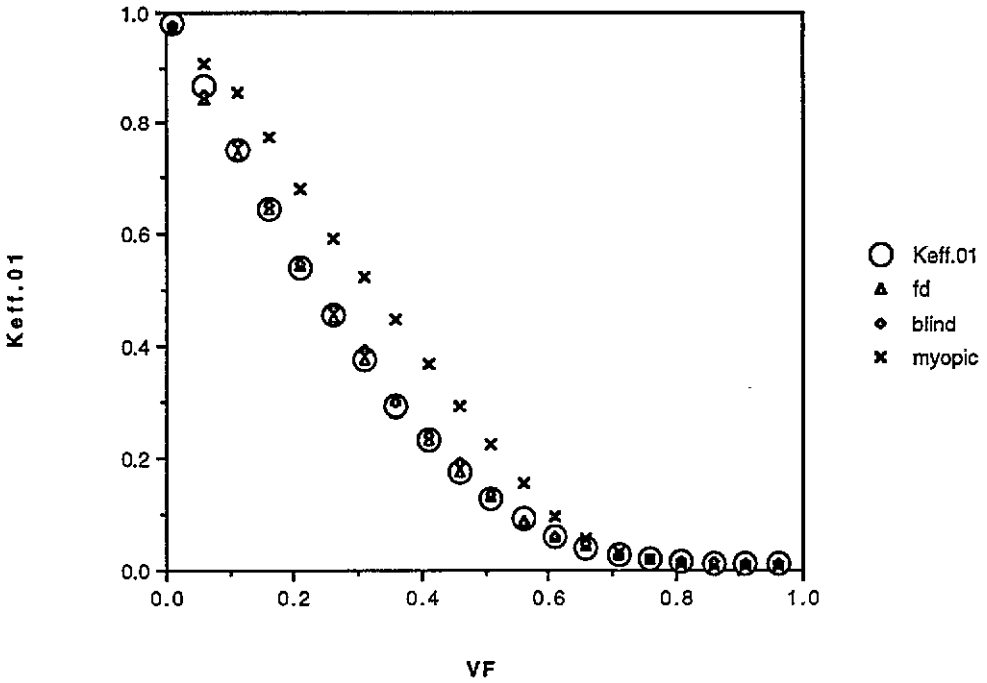

Figure 1. Effective permeability versus volume fraction for a random, uncorrelated, two-component system with a permeability contrast ratio of 0.01. Comparison between the CTRW algorithm (K_{eff} 0.01, ○), the blind ant algorithm (□), the myopic ant algorithm (×), and a finite-difference algorithm (△). In all cases, the error bars are of the order of twice the size of the plotting symbols used and have been omitted for clarity.

How the time-scale is chosen depends on the type of permeability distribution being simulated and the required accuracy. For a discrete two-component distribution, or for a continuous uniform distribution, it is sufficient to use walks with a maximum time of 10^3 units to get answers correct to two significant figures. This is illustrated by the results shown in table 1 for effective permeability calculations on four continuous uniform distributions. The table compares results obtained using a finite-difference algorithm with those obtained using the CTRW method with different maximum times. Statistics were taken over 10 realizations of the permeability distribution on a lattice of size 30^3, with 1000 random walkers on each realization.

Table 1 also contains values of the arithmetic and geometric means of the distributions. For continuous uniform distributions, the geometric mean is a very good estimator of the effective permeability. Other analytical estimators, e.g. from perturbation theory, are also good in this case. However, they break down in the case of two-component distributions with a large permeability contrast ratio (i.e. sandstone–shale distributions), or lognormal distributions with a large variance [12]. The random-walk method can handle these awkward cases.

Figure 1 shows graphs of effective permeability versus volume fraction calculated for random, uncorrelated, two-component systems with a permeability contrast ratios of 0.01. The figure compares results obtained using the CTRW algorithm with those obtained using the blind ant algorithm [6], the myopic ant algorithm [18], and a finite-difference algorithm. The random walks were of length 1000 steps. It is clear that the different methods give consistent results, except for the myopic ant algorithm.

Table 2. CPU times taken to calculate the permeability for ten realizations of a random, uncorrelated, two-component system with a permeability contrast ratio of 0.01 and a shale volume fraction of 0.4. Comparison of finite-difference and CTRW methods of an Apollo 10 000 workstation.

Lattice size	Method	CPU time (s)
30^3	Finite difference	1 285.4
30^3	CTRW (1000 steps)	258.6
100^3	Finite difference	138 998.8
100^3	CTRW (1000 steps)	914.0
100^3	CTRW (10 000 steps)	3 193.5

Table 3. Results for lognormal distribution $[a, b, c]$, where a is the geometric mean, b is the variance and $\exp(c)$ is the high-permeability cut-off. Comparison of finite differences (FD) with CTRW algorithm for various maximum times.

	[2, 0.5, 80]	[2, 10, 8]	[2, 10, 80]
Arithmetic mean	2.6	59	304
Geometic mean	2	2	2.
Maximum permeability	20	3000	60 000
Estimsted time-scale	8000	50 000	200 000
K (FD)	1.943 ± 0.009	2.356 ± 0.058	2.469 ± 0.40
K (CTRW) 10^3 steps	1.92 ± 0.05		
K (CTRW) 10^4 steps	1.95 ± 0.06	2.53 ± 0.10	3.77 ± 0.44
K (CTRW) 10^5 steps	1.95 ± 0.05	2.34 ± 0.05	2.71 ± 0.17
K (CTRW) 10^6 steps			2.43 ± 0.11

Table 2 shows CPU times taken to calculate the permeability for ten realizations of a random, uncorrelated, two-component system with a permeability contrast ratio of 0.01 and a shale volume fraction of 0.4. The comparison is between the finite-difference and CTRW methods on an Apollo 10 000 workstation. The method used for matrix inversion in the finite-difference method was conjugate gradients without preconditioning. These times indicate the greater efficiency of the CTRW method, especially as the lattice size increases. However, the question of efficiency is not an easy one to pin down. It is complicated by the fact that the length of the walks in the CTRW method is not fixed, but depends on the path taken. Also, in general, the random-walk method can only be expected to give 5–10% accuracy [23] because of its intrinsic noisiness, whereas the finite-difference method can be made to converge to an arbitrary accuracy for a well posed problem. The random-walk method comes into its own when the size of the lattice precludes the use of finite differences. An accuracy of 5–10% is quite acceptable for problems of the type addressed in this paper (i.e. calculating the permeability of porous media).

Table 3 shows the results obtained for three lognormal distributions with different variances and/or high-permeability cut-offs. The estimated time-scale for the CTRW algorithm is calculated from the ratio of the maximum permeability value to the arithmetic mean, multiplied by 1000. This compensates for the normalization of the bond probabilities which must be carried out in order to make the values lie in the interval $[0, 1/z]$. The estimated time-scales are validated by the convergence of the effective permeability results in table 3. Referring to the details of the CTRW algorithm, it is clear that the time taken for the simulations is not directly proportional to the maximum number of time steps, since a walk can terminate at any step if the updated time is greater than the maximum time. It depends on the distribution of bond connectivites.

6. Other applications

The CTRW method is not restricted to regular lattices. It can easily be implemented on random lattices such as an unstructured Delaunay mesh [25]. This suggests an application of the method to calculating the conductivity of tortuous porous systems [23]. An unstructured mesh could be constructed inside the porous region, with its nodes distributed densely inside narrow pores, and appropriate bond connectivites assigned using standard finite-difference techniques [9]. Then random walkers would be allowed to diffuse through the system according to the CTRW rules. Using an unstructured mesh ensures that the random walkers move relatively large distances when far from a boundary and short distances when near a boundary. Using the CTRW method enables the heterogeneous bond connectivities to be dealt with in an efficient manner.

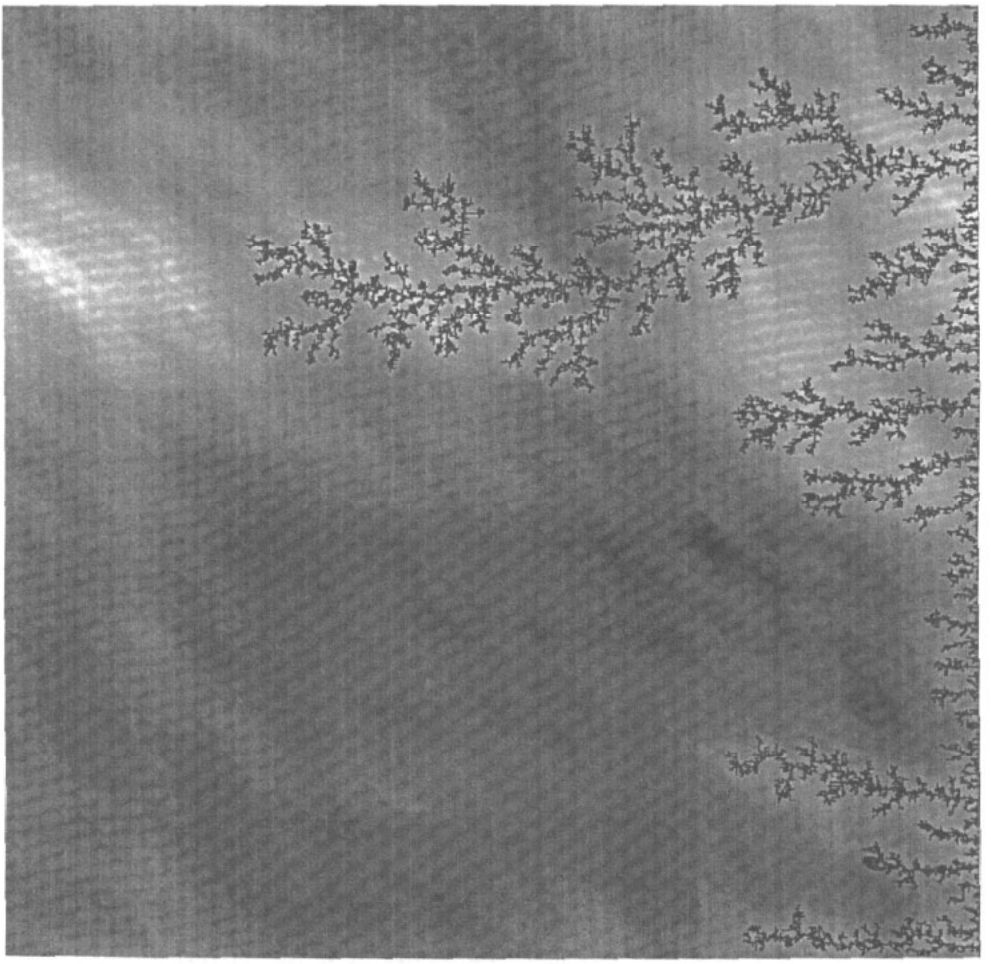

Figure 2. DLA on a fractal map of permeability.

The CTRW method can easily be applied to diffusion-limited aggregation (DLA) in random media. In DLA, only the endpoint of the walk is important, not the time taken. Therefore, it would only be necessary to choose which neighbour to move to at each simulation step, not

to update the time. In this case, the method reduces to that of Selinger *et al* [21]. Figure 2 shows the result of a DLA process carried out in a region of fractal permeability using the CTRW method. The fractal map was generated using the fast fourier transform technique of Voss [24]. Note that the cluster tends to move into the regions of high permeability (i.e. lightly shaded regions).

Another application of CTRW in random media is in determining connected regions of high permeability between wells in geological models of petroleum reservoirs [17].

7. Conclusion

In this paper a CTRW method has been introduced for applications to transport processes in random media. The method is efficient and is easily parallelizable, which will be an important consideration in the emerging era of parallel computing. The method can be used to calculate the diffusivity of homogeneous mixtures of many components, with applications to effective permeability and conductivity measurements. It is also applicable to DLA in random media and to determining connected regions of high permeability in geological models of petroleum reservoirs.

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