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Particle tracking for fractional diffusion with two time scales

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ABSTRACT

Previous work [Y. Zhang, M.M. Meerschaert, B. Baeumer, Particle tracking for time-fractional diffusion, Phys. Rev. E 78 (2008) 036705] showed how to solve time-fractional diffusion equations by particle tracking. This paper extends the method to the case where the order of the fractional time derivative is greater than one. A subordination approach treats the fractional time derivative as a random time change of the corresponding Cauchy problem, with a first derivative in time. One novel feature of the time-fractional case of order greater than one is the appearance of clustering in the operational time subordinator, which is non-Markovian. Solutions to the time-fractional equation are probability densities of the underlying stochastic process. The process models movement of individual particles. The evolution of an individual particle in both space and time is captured in a pair of stochastic differential equations, or Langevin equations. Monte Carlo simulation yields particle location, and the ensemble density approximates the solution to the variable coefficient time-fractional diffusion equation in one or several spatial dimensions. The particle tracking code is validated against inverse transform solutions in the simplest cases. Further applications solve model equations for fracture flow, and upscaling flow in complex heterogeneous porous media. These variable coefficient time-fractional partial differential equations in several dimensions are not amenable to solution by any alternative method, so that the grid-free particle tracking approach presented here is uniquely appropriate.

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1. Introduction

Time-fractional diffusion equations are related to continuous time random walk (CTRW) stochastic processes with infinite-mean waiting times between particle jumps. When $0 < \gamma < 1$, a random waiting time W with a power-law probability tail $P(W > t) \sim t^{-\gamma}$ has an infinite mean, and this leads to a time-fractional derivative of the same order. See, for example, the extensive review articles of Metzler and Klafter [1,2]. Power-law waiting times with tail index $\gamma > 1$ are also commonly observed, including the wait between solar flares [3], wait between doctor visits ($\gamma \approx 1.4$) [4], wait between large price returns in the stock market ($\gamma > 1$) [5], wait between earthquakes ($\gamma = 1.13$ [6] and 1.66 [7]), and wait between movement of contaminants in heterogeneous porous media ($\gamma \geq 1$ [8] and $\gamma \approx 2$ [9]). Recent work of Baeumer et al. [10,11] and Becker-Kern et al. [12] extends the time-fractional diffusion equation and its underlying CTRW model to the case $1 < \gamma \leq 2$. Since a power-law waiting time with tail index γ has a positive finite mean, a two-scale limit procedure is employed. The governing equation involves both a first derivative in time, and another time derivative of order γ. In case of variable coefficients, analytical solutions are unavailable, motivating the development of numerical solvers.

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This study develops a particle tracking method for time-fractional diffusion equations (FDE) of order $1 < \gamma \leq 2$. The grid-free Lagrangian solver is computationally more efficient than Eulerian approaches in solving realistic diffusions with multiple dimensions and fine-scale details (for example, see [13–16]). The Lagrangian solution also reveals the dynamics of particles undergoing complex diffusive process [17,18], and is the only viable solution method in some cases [19].

Particle tracking solutions for fractional diffusion equations with time derivative of order $0 < \gamma < 1$ have been considered recently by several authors [20–28,19]. These models are typically limited to a fractional time derivative of index $0 < \gamma \leq 1$ [29–36]. The underlying CTRW model imposes a random waiting time $W_i > 0$ before each random particle displacement X_i. If $P(W_i > t) \sim t^{-\gamma}$ with $0 < \gamma < 1$ then the sum $T_n = W_1 + \cdots + W_n$ gives the time of the nth particle jump, and the particle location at this time is $S_n = X_1 + \cdots + X_n$. In the scaling limit, the random walk of particle jumps converges to a limit process, a Brownian motion if each X_i has zero mean, and finite variance. The random walk of jump times also converges: $c^{-1/\gamma} T_{[cm]} \Rightarrow D(m) \geq 0$ via the extended central limit theorem (CLT) for infinite variance summands [32,37]. The number of particle jumps $N(t)$ by time $t > 0$ is an inverse process $\{T_n \leq t\} = \{N(t) \geq n\}$ with an inverse scaling limit $c^{-\gamma} N([ct]) \Rightarrow E(t)$ where $\{E(t) \leq m\} = \{D(m) \geq t\}$.

Typically the random walk of particle jumps has a Brownian motion scaling limit $c^{-1/2} S_{[ct]} \Rightarrow A_t$. Then the CTRW particle location $S_{N(t)}$ at time $t > 0$ has scaling limit $c^{-\gamma/2} S_{N(ct)} \Rightarrow A_{E(t)}$ with the time index replaced by the non-Markovian inverse stable subordinator $E(t)$. The probability density function $u(x, t)$ of the CTRW scaling limit $x = A_{E(t)}$ solves a time-fractional diffusion equation $(\partial/\partial t)^\gamma u = Lu$ where the Caputo derivative in time is used, and the spatial derivative operator is $L = \mathcal{D}\partial^2 u/\partial x^2$, see [37]. Particle tracking codes for time-fractional diffusion equations with $0 < \gamma < 1$ trace the path of a particle $A_{E(t)}$ over time and space. One alternative is to simulate the CTRW, but simulation of the limit process is more efficient and more accurate. A useful observation is that $x = A_m$ and $t = D(m)$ are Markov processes in the operational time variable m, leading to a very efficient code [19].

If particle jumps X_i have a nonzero mean, the traditional CLT requires that the mean jump undergoes linear rescaling, and the deviation from the mean is subject to square root rescaling. The resulting random walk limit for the particle jumps is a Brownian motion with drift, and the time-fractional diffusion equation uses $Lu = -v\partial u/\partial x + \mathcal{D}\partial^2 u/\partial x^2$. Note that the two spatial scales result in two x-derivative terms. If particle jumps have a power-law probability tail $P(X_i > x) \sim r^{-\alpha}$ then the random walk limit for the particle jumps is an α-stable Lévy motion, and the space-fractional operator appears: $Lu = \mathcal{D}\partial^\alpha u/\partial x^\alpha$. A large class of time-fractional diffusion equations of the form $(\partial/\partial t)^\gamma u = Lu$ can be solved by particle tracking, using an appropriate particle motion process A_m corresponding to L, and the same $E(t)$ subordinator [19].

If $1 < \gamma \leq 2$ then the subordinator in the CTRW limit is more complicated: the mean wait and the deviation from that mean have to be normalized separately [12]. The time limit process is a γ-stable Lévy motion with positive drift $D(m)$, its mean exists since $\gamma > 1$, and there is a small probability that $D(m) < 0$. Of course there are no negative waiting times, but there are short waiting times less than the mean, the deviation is negative, and these can accumulate in the limit [12]. Rescaled CTRW waiting times can be positive or negative, since the mean is subtracted. If τ_i is the sum of the first i rescaled waiting times, then $T_n = \max\{\tau_1, \ldots, \tau_n\}$ represents the time of the nth particle jump. The effect is that particle jumps cluster, with a random cluster size equal to the number of consecutive negative rescaled waiting times. The $N(t)$ scaling limit is $M(m) = \sup\{D(m') : 0 < m' < m\}$ with inverse process $E(t)$, and the CTRW scaling limit is again $A_{E(t)}$. The two time scales lead to a fractional diffusion equation that involves a pair of time derivative terms.

This paper develops a particle tracking code for time-fractional diffusion equations with $1 < \gamma \leq 2$. The code tracks particles $A_{E(t)}$ over time and space by simulating $x = A_m$ and $t = M(m)$ in operational time, extending the approach of [19]. One added complication is that the operational time $t = M(m)$ is no longer Markovian. However, since it is the supremum of the Markov process $D(m)$, it can be efficiently simulated. Section 2 develops the Lagrangian particle tracking approach, by developing the Langevin equations for the underlying Markov processes. Numerical verifications are given thereafter in Section 3. In Section 4, the code is applied to space–time-fractional groundwater flow equations in multiple dimensions, which cannot be solved by other known methods. This also demonstrates the ability of these equations to model upscaled solute transport for complex heterogeneous porous media. Finally some conclusions are summarized in Section 5.

2. Stochastic process model for particle tracking

Particle tracking codes depend on the relationship between fractional diffusion equations and the underlying stochastic processes. Meerschaert and Scheffler [38] show that the random walk of particle jumps has a scaling limit $x = A_m$ whose probability density $p(x, m)$ has Fourier transform $\hat{p}(k, m) = \mathrm{e}^{m\hat{L}(k)} = \int \mathrm{e}^{-\mathrm{i}kx} p(x, m)\mathrm{d}x$. Here $\hat{L}(k)\hat{p}$ is the Fourier transform of Lp. For example, if the random walk has jumps with mean zero and finite variance, the scaling limit $x = A_m$ is a Brownian motion, its Gaussian probability densities $p(x, m)$ solve a diffusion equation $\partial p/\partial m = Lp$ with $L = \mathcal{D}\partial^2/\partial x^2$, and $\hat{L}(k) = -\mathcal{D}k^2 = \mathcal{D}(\mathrm{i}k)^2$. Then $\hat{p}(k, m) = \mathrm{e}^{-m\mathcal{D}k^2}$ and the diffusion equation follows from inverting $\mathrm{d}\hat{p}/\mathrm{d}m = \hat{L}(k)\hat{p}$, using the fact that $(\mathrm{i}k)\hat{p}$ is the Fourier transform of $\partial p/\partial x$. If particle jumps X_i have a nonzero mean, the traditional CLT requires two scales, one for the mean and another for deviations from the mean. The random walk limit $x = A_m$ is a Brownian motion with drift, and the governing equation uses $L = -v\partial/\partial x + \mathcal{D}\partial^2/\partial x^2$. Note that the two spatial scales result in two x-derivative terms. For random walk jumps with a power-law probability tail $P(X_i > x) \sim x^{-\alpha}$ where $0 < \alpha < 2$, the scaling limit is an α-stable Lévy motion $x = A_m$. Its density has Fourier transform $\hat{p}(k, m) = \mathrm{e}^{m\hat{L}(k)}$ where $\hat{L}(k) = \mathcal{D}(\mathrm{i}k)^\alpha$, so that

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$L = \mathcal{D}\partial^\alpha/\partial x^\alpha$ and the density solves a fractional diffusion equation $\partial p/\partial m = Lp$. If the heavy tailed jumps have a nonzero-mean value, then a two-scale limit leads to an α-stable Lévy motion with drift, whose Fourier symbol $\hat{L}(k) = -v(\mathrm{i}k) + \mathcal{D}(\mathrm{i}k)^\alpha$ corresponds to the space-fractional diffusion operator $L = -v\partial/\partial x + \mathcal{D}\partial^\alpha/\partial x^\alpha$.

Becker-Kern et al. [12] show that, when waiting times between particle jumps have a power-law tail $P(W_i > t) \sim t^{-\gamma}$ for $1 < \gamma \leq 2$, the scaling limit $t = D(m)$ for the random walk of waiting times has probability density function $g(t, m)$ with Fourier transform $\hat{g}(\lambda, m) = \mathrm{e}^{-m\psi(\lambda)} = \int \mathrm{e}^{-\mathrm{i}\lambda t} g(t, m)\mathrm{d}t$. Here $\psi(\lambda) = \mathrm{i}\lambda - a(\mathrm{i}\lambda)^\gamma$ so that $\mathrm{d}\hat{g}/\mathrm{d}m = -\psi(\lambda)\hat{g} = -(\mathrm{i}\lambda)\hat{g} + a(\mathrm{i}\lambda)^\gamma\hat{g}$. This inverts to

$$\frac{\partial g(t, m)}{\partial m} = -\frac{\partial g(t, m)}{\partial t} + a\frac{\partial^\gamma g(t, m)}{\partial t^\gamma} \tag{1}$$

where $\partial^\gamma g/\partial t^\gamma$ is the Riemann–Liouville fractional derivative, which can be defined as the inverse Fourier transform of $(\mathrm{i}\lambda)^\gamma\hat{g}$. The point source initial condition $\hat{g}(\lambda, m) \equiv 1$ ensures that $D(0) = 0$ with probability one. The inverse process $E(t) = \inf\{m > 0 : M(m) > t\}$ where $M(m) = \sup\{D(m') : 0 \leq m' \leq m\}$ as explained in Section 1. A lengthy Laplace transform argument in Baeumer et al. [10] shows that the probability density $h(m, t)$ of the inverse process $m = E(t)$ solves

$$\frac{\partial}{\partial m}h(m, t) = -\frac{\partial h(m, t)}{\partial t} + a\left(\frac{\partial}{\partial t}\right)^\gamma h(m, t) + \delta(t)f(m) \tag{2}$$

where the Caputo fractional derivative $(\partial/\partial t)^\gamma h(m, t)$ is the inverse Laplace transform of $s^\gamma\tilde{h}(m, s) - s^{\gamma-1}h(m, 0)$ and $\tilde{h}(m, s) = \int_0^\infty \mathrm{e}^{-st}h(m, t)\mathrm{d}t$. The boundary condition $f(m)$ in operational time is uniquely determined by a, γ, see Baeumer et al. [10,11] for more details.

The probability density $u(x, t)$ of CTRW limit process $x = A_{E(t)}$ can be computed by conditioning:

$$u(x, t) = \int_0^\infty p(x, m)h(m, t)\mathrm{d}m \tag{3}$$

where t denotes clock time, and m denotes operational time. Informally, Eq. (3) expresses $P(A_{E(t)} = x) = \sum_m P(A_m = x)P(E(t) = m)$ as a sum over operational time. The first term under the sum models particle motion in the absence of any delays. The second is the operational time. The operational time density $h(m, t)$ in (3) acts as a transfer function that accounts for the time a particle spends in motion [39,40], so that the density $u(x, t)$ at clock time t is a weighted average of densities $p(x, m)$ at each operational time m. The operational time process $m = E(t)$ links the clock time t and its operational time counterpart m via the time-subordination principle [10,32,41]. Becker-Kern et al. [12] and Baeumer et al. [10] show that the density $u(x, t)$ of the CTRW scaling limit $x = A_{E(t)}$ solves

$$-a\left(\frac{\partial}{\partial t}\right)^\gamma u(x, t) + \frac{\partial u(x, t)}{\partial t} = Lu(x, t) + r(x)\delta(t) \tag{4}$$

with a point source initial condition, where $(\partial/\partial t)^\gamma$ is the Caputo fractional derivative, and $r(x)$ depends only on a, γ, and L. To reconcile (4) with (2) simply note that $L = -\partial/\partial x$ corresponds to the simplest (time-fractional wave equation) case $x = A_m = m$.

The Lagrangian approximation of the motion process $x = A_m$ for classical diffusion $L = D\partial^2/\partial x^2$ is well known. For space-fractional diffusion, the correct Lagrangian form has been given recently by Zhang et al. [42,43]. It remains to develop a Lagrangian approximation for the operational time process $m = E(t)$. Our approach is similar to the case of a time-fractional diffusion with $0 < \gamma < 1$, which was addressed in [19]. Recall from Section 1 that the operational time process is the inverse to the maximum process $M(m) = \sup\{D(m') : 0 < m' < m\}$, where $D(m)$ is the scaling limit of the random walk of waiting times. Then $D(m)$ is a Markov process, for which we can develop a Langevin equation. The probability density $g(t, m)$ of the γ-stable Lévy motion $t = D(m)$ solves the fractional diffusion equation (1). Since this equation has exactly the same form as the space-fractional diffusion equation considered in [42,43], we can use the same mathematical approach to obtain the Langevin stochastic differential equation for this Markov process. Following the same argument as in [42], we find that (1) is the forward equation for the Markov process

$$\mathrm{d}T = \mathrm{d}m + \mathrm{sign}\left(-a\cos\frac{\pi\gamma}{2}\right)\mathrm{d}w, \tag{5}$$

where the second term on the RHS is a rescaled stable random noise

$$\mathrm{d}w = \left(-a\mathrm{d}m\cos\frac{\pi\gamma}{2}\right)^{1/\gamma} S_\gamma(\beta^* = +1, \sigma = 1, \mu = 0), \tag{6}$$

and the sign function $\mathrm{sign}(\chi) = +1$ if $\chi \geq 0$, otherwise -1. $S_\gamma(+1, 1, 0)$ is a standard stable random variate in the Samorodnitsky and Taqqu [44] parameterization (with β^*, σ, and μ denoting the skewness, scale, and shift, respectively). Note that the random process $t = D(m)$ is the sum of $\mathrm{d}T$ at each jump. Since the sign function in (5) is always $+1$, the Time-Langevin equation (5) simplifies to

$$\mathrm{d}T = \mathrm{d}m + \mathrm{d}w. \tag{7}$$

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If dT is regarded as the waiting time during each jump, then (7) shows that the waiting time can be separated into two parts: the mean wait (dm) and the deviation from the mean (dw). The deviation dw is negative if the γ-stable noise S_γ is negative.

The simplified Time-Langevin equation (7) is analogous to the case $0 < \gamma < 1$ (take $b = 0$ in (6) of [19]). When $0 < \gamma < 1$, the mean of the stable is undefined, the dm disappears, and $dw = dT$. The main difference is that we always have $dw > 0$ when $\gamma < 1$, so that we can compute the inverse process more simply. In the present case where $\gamma > 1$, we need one extra step. We begin by simulating the Langevin sample path (7) to get $T_i = \sum_{j\le i} dT_j$ where $dT_j = dm_j + dw_j$. The increments $dm_j = dm$ are all equal steps in operational time. The dw_j are simulated stable random variables with mean zero and index γ following (6). To get the inverse, we first compute the maximum $t_i = \max\{T_1, \ldots, T_i\}$. Then $t_i = M(m_i)$ where $m_i = i\,dm$ in equal operational time steps. The inverse process $m_i = E(t_i)$ in unequal, random increments of clock time whose length depends on the random dw_i. In a similar manner, we follow the Langevin approach in [42] to get $x_i = A_{m_i}$ for the same equally spaced steps in operational time. Then the points (t_i, x_i) trace out the graph of the random sample path $x = A_{E(t)}$ as required. To summarize, the Lagrangian framework to approximate (4) contains the following four steps:

Step 1. Calculate dT_i based on a pre-defined operational time step dm. First, use (6) to generate the random number dw_i. Then use (7) to get dT_i.

Step 2. Calculate the particle jump dX_i (a vector for the multiple dimension FDE) in the operational time dm. Note that the particle movement in operational time is Markovian. Examples will be shown in the next two sections.

Step 3. Repeat Steps 1 and 2, and compute $T_i = \sum_{j\le i} dT_j$ and $x_i = \sum_{j\le i} dX_j$. Then let $t_i = \max\{T_1, \ldots, T_i\}$.

Step 4. Output particle location x_i at the corresponding clock time t_i.

By repeating the four steps until $t_i \ge T_{\text{end}}$ for a large number of particles, and then creating a histogram of the results, we obtain a solution of the time-fractional diffusion equation (4) when $1 < \gamma \le 2$. Since the clock time points are random, it is necessary to interpolate to obtain the solution at any given time point t. This Lagrangian framework marches forward in both time and space, as a function of the synthetic variable, operational time.

3. Operational time density

Numerical tests were performed to validate the random walk particle tracking scheme developed in Section 2. We first consider particle tracking solutions to Eq. (2) for the operational time density $h(m, t)$, which can be compared to inverse Fourier transform solutions [10,11].

The Lagrangian solver developed above does not calculate the operational time density directly, but rather it simulates the sample path in operational time for each particle. Fig. 1(a), (b) illustrates the operational time simulation. The figure shows three realizations of the operational time process $m = E(t)$ for two different values of γ. Note the equal increments in the operational time variable, which was chosen to be rather large for purposes of illustration. The horizontal segments in the graph are caused by large positive jumps dw. The vertical segments occur when the increment $dT = dm + dw$ is negative, so that the max process stays constant. Although we plot $m_i = E(t_i)$ in the graphs, the simulation directly generates the process $t_i = M(m_i)$, and then the axes are inverted to reveal the inverse process. Fig. 1(c), (d) shows the simulated particle density from a histogram of 10,000 particles. The symbols are the particle tracking solutions of (2) and the curves are the semi-analytical solutions to the same equation, obtained by inverse Fourier transforms (IFT). It is apparent that the particle tracking solutions are in good agreement with the semi-analytical solutions.

Fig. 2 illustrates solutions of (2) for the special case $\gamma = 2$. Note that this is equivalent to solving the time-fractional diffusion equation (4) in the case $L = -\partial/\partial x$ which corresponds to $x = A_m = m$ (time-fractional wave equation). Here the generation of the stable random variable dw defined by (6) can be simplified as

$$dw = \xi\sqrt{2a\,dm}, \tag{8}$$

where ξ is a uniform random number with mean zero and variance 1. The summation of dw is approximately Gaussian. As a further check, we repeated this experiment with a normally distributed random variable dw with zero mean and unit variance, using the function "gasdev" in [45] (page 280). No improvement was apparent (examples are not shown here), and thus we suggest using (8), which is somewhat more efficient.

4. Applications

To further investigate the applicability, flexibility, and efficiency of the Lagrangian solver for real diffusive process, we apply particle tracking to simulate solute particle transport through heterogeneous porous media and fractured aquifers.

4.1. Case 1: Solute transport in 2D fracture networks

Ensemble solute transport through 2D regional-scale discrete fracture networks can be characterized by a space and time FDE model, as concluded by Reeves et al. [46]. Large jumps occur for particles traveling along interconnected, high-permeable fractures, while the particles can also be trapped in the surrounding low-permeable matrix. An efficient simulator

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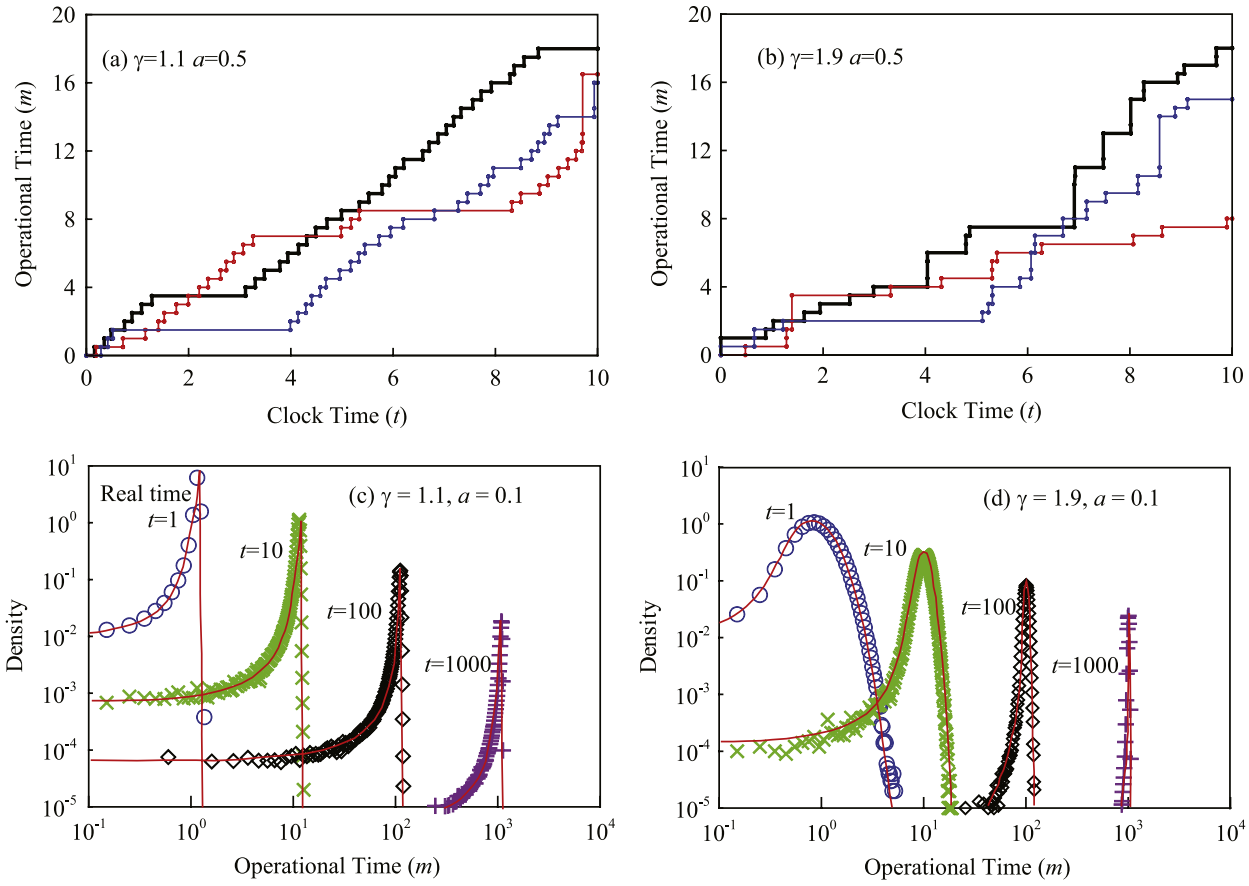

Fig. 1. Graphs (a) and (b) show three sample paths of the operational time process $m = E(t)$. For illustration purpose, a large operational time step dm is used. Graphs (c) and (d) show the density $h(m, t)$ of operational time computed via particle tracking (symbols) and inverse Fourier transforms (lines).

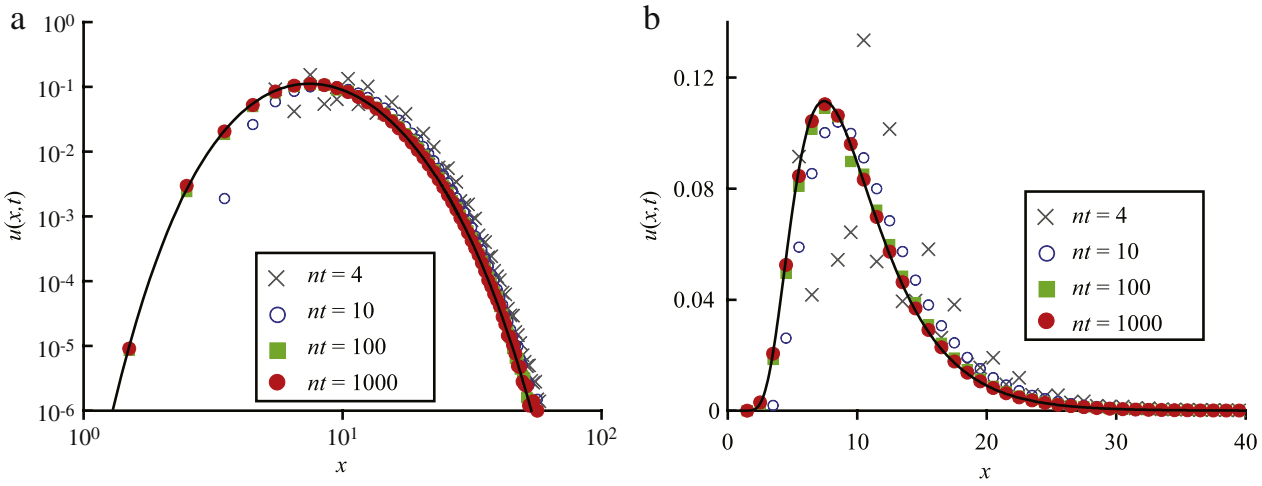

Fig. 2. Particle tracking solution (symbols) versus IFT solution (lines) for the FDE (4) with $L = -\partial/\partial x$ and $\gamma = 2$ at $t = 10$. Graph (b) is the linear–linear plot of (a). The variable nt is the total number of time steps.

for such combined super- and sub-diffusive process is needed. We propose the following multiscaling FDE:

$$\left(-a\frac{\partial^\gamma}{\partial t^\gamma} + \frac{\partial}{\partial t}\right) u(\vec{x}, t) = \mathcal{D}\nabla^{H^{-1}}_{M(\mathrm{d}\theta)} u(\vec{x}, t) + r(\vec{x})\delta(t), \tag{9}$$

where $\mathcal{D}$ is the dispersion coefficient, H is the scaling matrix, and $M(\mathrm{d}\theta)$ is the mixing measure [43]. The operator on the right-hand side is a multiscaling fractional derivative in space, see Schumer et al. [47]. In short, the model assumes power-law particle jumps where $M(\mathrm{d}\theta)$ is the probability distribution of the radial jump direction, and the eigenvalues of H give the tail index α for jumps in the corresponding eigenvector direction, so that the probability of a jump longer than r in this

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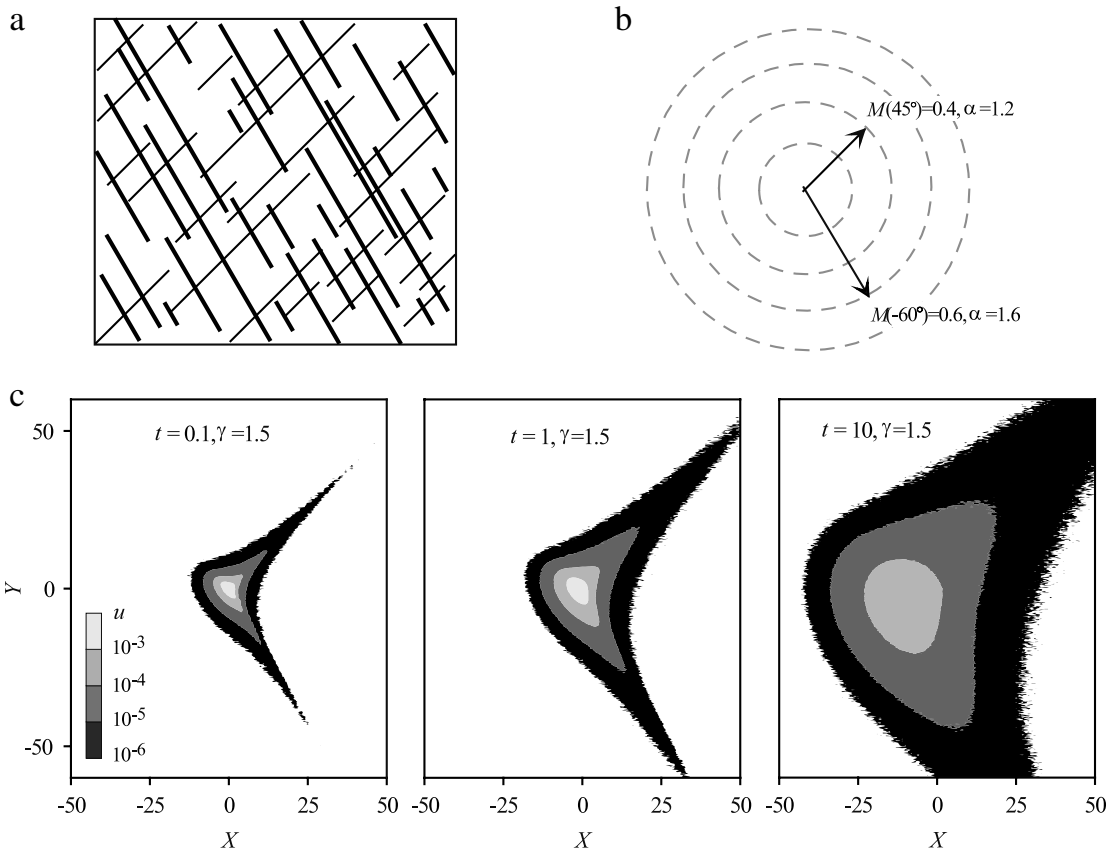

Fig. 3. Case 1: Conceptual model of a 2D fracture network (a), the corresponding model parameters (b), and particle tracking solutions (c) to the model equation (9) with $\gamma = 1.5$, $a = 0.5$, and $\mathcal{D} = 1$ at time 0.1, 1, and 10, respectively. Initial source location is (0, 0).

direction falls off like $r^{-\alpha}$ for r large. In the application to fracture flow, the mixing measure codes the fracture orientation, and the matrix H codes fracture length and aperture.

Step 2 of the Lagrangian solver is to simulate the particle jump process. The particle tracking code represents a random jump length in the radial direction $\mathrm{d}\theta_i$ during operational time step $\mathrm{d}m$ as [43]

$$R_i = \left(-\mathcal{D}\mathrm{d}m \cos\frac{\pi\alpha_i}{2}\right)^{1/\alpha_i} S_{\alpha_i}(1, +1, 0), \tag{10}$$

where α_i is the scale index of Lévy motion along angular $\mathrm{d}\theta_i$. The radial jump direction at each operational time step is randomized according to the mixing measure (for details, see [43]). This produces a suitable approximation of the underlying operator stable jump, see for example Meerschaert and Scheffler [48].

Fig. 3 illustrates a conceptual example application of this fracture flow model. The fracture network consists of two groups of fractures along different orientations (Fig. 3(a)), represented by two point masses in the mixing measure, as shown in Fig. 3b. The simulated 2D particle density u shows both the evolution of solute plume along the fractures and the retention of particles near the source (Fig. 3(c)).

Note the transport parameters in (9), including $\mathcal{D}$ and $M(\mathrm{d}\theta)$, can be space dependent, due to local variations in aquifer properties [9]. The jump size (10) can easily handle spatial variation of these parameters. We are not aware of any other numerical method that can solve equation (9) with spatially variable coefficients.

4.2. Case 2: Upscaling solute transport in heterogeneous porous media

A detailed Monte Carlo simulation was used to simulate a complex porous medium with regional-scale heterogeneity (facies) as well as small- to medium-scale heterogeneity in material properties and structure. The method used is the same as Zhang et al. [9], but here the actual spatial distribution of aquifer heterogeneity differs, since different model parameters are used. A classical advection–dispersion solver is used to obtain plume behavior in this simulated aquifer, and then we apply a much simpler upscaled fractional diffusion model that approximates the same plume behavior. This demonstrates the ability of fractional diffusion equations to simplify complex anomalous diffusion.

We built 100 different, equally possible, hydrofacies models representing a coarse-grain dominated alluvial system. Fig. 4 illustrates one such system. The transition probability geostatistics approach developed by Carle and Fogg [49, 50] was selected to generate the facies models. A 3D steady-state modeling approach was used to simulate velocity

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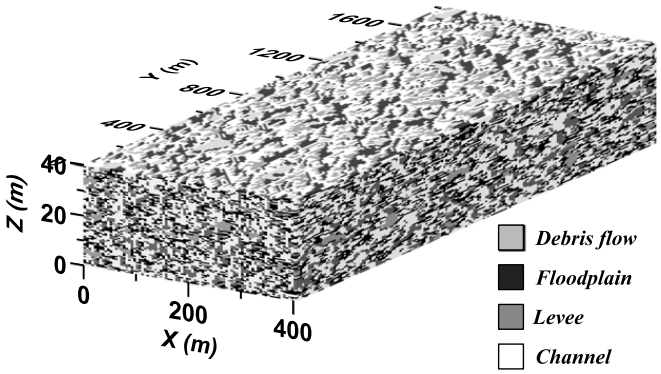

Fig. 4. 3D view of synthetic hydrofacies model. For visualization purpose, a different scale is used for each axis.

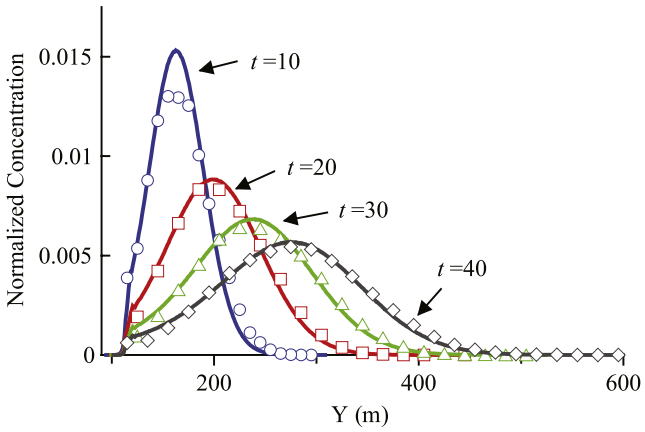

Fig. 5. Case 2: Plume concentration snapshots at $t = 10, 20, 30$, and 40 yr respectively, in the direction of flow. Detailed Monte Carlo numerical simulations (symbols) of the second-order advection–dispersion equation versus the best-fit Lagrangian approximations (lines) via the FDE (11) with $\gamma > 1$. The FDE is an upscaling model for the more complex Monte Carlo plumes. See the text for model parameters.

distributions in the aquifer with the finite difference code MODFLOW [51]. Transport simulations employed the random walk particle method described by LaBolle et al. [18,52]. The motion of particles was simulated by the classical, second-order advection–dispersion equation. Except for the hydrofacies models, the other set-up, including model boundary and initial conditions and flow and transport parameters, are the same as those used by Zhang et al. [9].

The simulated Monte Carlo particle concentration (after normalization) at each sampling cycle is the ensemble average of 100 realizations. The following time-fractional diffusion equation is then used to fit the Monte Carlo plumes along the longitudinal flow direction:

$$\left(-a\frac{\partial^\gamma}{\partial t^\gamma} + \frac{\partial}{\partial t}\right) u(x,t) = -\frac{\partial}{\partial x}\left[Vu(x,t) - \mathcal{D}\frac{\partial u(x,t)}{\partial x}\right] + r(x)\delta(t), \tag{11}$$

where constant velocity V and dispersivity $\mathcal{D}$ is used. Eq. (11) is an upscaling model that simplifies the complex structure of the synthetic aquifer, which would otherwise be represented by a highly complex velocity and dispersivity field.

The four-step Lagrangian algorithm from Section 2 was used to solve (11). Here the motion process in Step 2 is calculated by

$$\mathrm{d}X = V\mathrm{d}m + [2\mathcal{D}\mathrm{d}m]^{1/2}\,\xi \tag{12}$$

where ξ is a uniform random number with mean zero and variance 1.

The first snapshot along the longitudinal direction (or Y-axis in Fig. 4) at time 10 years provides the best-fit parameters $\gamma = 1.2, a = 9.0\,\mathrm{yrs}^{0.2}, V = 19\,\mathrm{m/yr}$, and $\mathcal{D} = 34\,\mathrm{m}^2/\mathrm{yr}$. The same values were then used in the upscaling equation (11) to model the remaining snapshots. Results show that the Lagrangian solutions of the model equation (11) provide a surprisingly good approximation to the Monte Carlo results (Fig. 5). We conclude that the time-fractional diffusion equation provides a simple and accurate predictive model for upscaling plume behavior in complex aquifers that exhibit heterogeneity at multiple scales. In this application, the time-fractional derivative models a power-law waiting time $P(W > t) \sim t^{-\gamma}$ for particle retention.

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5. Conclusions

A diffusion equation with a fractional time derivative of order $1 < \gamma \leq 2$ governs the scaling limit of a decoupled continuous time random walk (CTRW) with power-law waiting times. The CTRW scaling limit can be decomposed into a motion process and an operational time process. Each process can be simulated by building a Langevin equation, and the combination results in a fully Lagrangian solver of the time FDE. Resting periods of the operational time process correspond to simultaneous particle jumps in the underlying CTRW. The resulting particle tracking code for time-fractional diffusion equations of order $1 < \gamma \leq 2$ is validated against semi-analytical inverse Fourier transform solutions, in the simplest cases where these alternative solution methods are viable. Illustrative applications demonstrate the ability of this time-fractional diffusion equation and its random walk approximation to model multidimensional fracture flow, and to provide a simpler approximation for upscaling flow and transport in complex porous media with heterogeneities at multiple scales.

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