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## Chapter for Handbook of Fractional Calculus with Applications

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# Particle tracking

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**Abstract:** This chapter reviews the Lagrangian solvers developed in the last two decades for fractional differential equations (FDEs). Both the Langevin approach and the fractional Lévy motion define dynamics of random walkers, whose density solves the FDE. For the vector FDEs, a multiscaling compound Poisson process can track trajectory of particles moving along arbitrary directions with direction-dependent scaling rates. Random walk particle tracking (RWPT) schemes, including streamline projection and flow subordination, are also needed to track particles whose mechanical dispersion follows streamlines. Particle paths affected by boundaries can also be modeled using RWPT, leading to a fully Lagrangian approximation for the vector spatiotemporal FDEs with streamline-dependent superdiffusion in domains of any size and boundary conditions, as required by real-world applications.

**Keywords:** Fractional differential equation, Lagrangian, Random walk particle-tracking

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## 1 Introduction

Fractional differential equations (FDEs) built upon fractional calculus, a mathematical tool initiated by Leibniz and Liouville [22, 24], have been proposed by the physics community and remain as an active area of research to simulate the ubiquitous anomalous diffusion for three decades [20, 21]. The FDEs use fractional derivative in time or space to capture the extremely long-term correlation of individual particle waiting times and/or motions. Analytical solutions are not available for most FDEs, motivating the development of numerical methods. Among these numerous methods, the Lagrangian solver built upon random walk particle-

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tracking (RWPT) is relatively new and exhibits promising applicability in the Earth sciences, where many geological materials, such as water, chemicals, sediment, rocks, soil, and glacial, can be represented by “particles”.

RWPT yields a grid-free, fully Lagrangian solution by simulating sample paths of the underlying stochastic process for the target material without modifying (such as truncating or discretizing) the governing equation. Solutions to constant coefficient FDEs are Lévy motions, whose  $\alpha$ -stable densities [26] are the scaling limits of random walks with power-law transition probabilities [19]. Hence, by tracking the trajectory of random-walking particles whose jump sizes and/or waiting times follow heavy tailed distributions, one solves the FDE. RWPT increases computational efficiency for large-scale flow systems with fine mesh [28], overcomes grid-average error for simulating a sharp density front [12], retains minimal numerical dispersion [11], has easy implementation, and near linear scaling on parallel computers, due to computational expense that depends on independent particle numbers rather than grid dimensions [9]. Most importantly, RWPT decomposes real-world dynamics into major components of particle jumps, which helps interpret the driving mechanisms, estimate effective parameters in a parsimonious model, and understand better the nature of the complex process. These advantages of the Lagrangian solver have motivated the recent development of particle-based approximations for the FDEs.

This study reviews the fundamental methodology of Lagrangian approximations for FDEs in the last two decades. Future research directions for the Lagrangian solver will also be identified. During the review, we will also focus on RWPT required by hydrological applications. The solid Earth system contains multi-scale heterogeneity, which motivates various heavy-tailed dynamics and provides an ideal base for the application of FDEs. Many moving targets in the Earth sciences can be regarded as particles, whose trajectories and dynamics can be described by the RWPT following specific FDEs [36].

## 2 Random walk particle tracking schemes

### 2.1 History and RWPT for 1-*d* FDEs

The RWPT has a long history in solving the advection-dispersion equation (ADE) by hydrologists to describe pollutant transport in aquifers [1, 12, 27, 29]. Other random walk methods developed by computational physics and engineering communities include lattice gas and lattice Boltzmann approaches, the use of particles for numerical thermodynamics, stochastic properties of perfect gases, and molec-

ular simulations in theoretical chemistry, which usually focus on different scales and will not be discussed here. Random walk solutions of the ADE typically depends on an analogy between the ADE and the forward equation for the associated Markov process. The forward equation, which provides a Lagrangian description of particles moving under specific Markov processes, is usually derived by the Langevin approach [25].

The Langevin approach is the first grid-free, formal Lagrangian solver developed to approximate the one-dimensional (1- $d$ ) space FDE with constant or continuous parameters [30], after the pioneer work of Chechkin and co-workers [3, 4], who modeled 1- $d$  fractional Lévy motion using random walkers, and Gorenflo et al. [6], who proposed a discrete random walk model after replacing the space/time FDEs by finite-difference equations. Gorenflo et al. [7, 8] then extended their discrete random walk model to a 1- $d$  continuous time random walk (CTRW) model, by subordinating the random walk to a renewal process. Marseguerra and Zoia [14, 15, 16] developed a Monte Carlo approach to model sub-diffusion across a discontinuity of parameters in 1- $d$ . Zhang et al. [33] developed an empirical reflection scheme to track particles undergoing super-diffusion across an interface with discontinuous parameters. Heinsalu et al. [10] developed a CTRW scheme for the 1- $d$  time fractional Fokker-Planck equation (FFPE). Magdziarz and Weron [13] developed a robust Monte Carlo approach to solve the 1- $d$  spatiotemporal FFPE. A brief review of the Langevin approach for 1- $d$  space and time FDEs is given in Appendix A.

## 2.2 Compound Poisson process for solving vector FDE

Many real-world transport problems require a vector FDE with variable parameters and multiscaling spreading rates, motivating the multi-dimensional RWPT approach based on the compound Poisson process [31, 32]. The multiscaling, fractional advection-dispersion equation (FADE) takes the form [17]:

$$\left( b \frac{\partial}{\partial t} + \beta \frac{\partial^\gamma}{\partial t^\gamma} \right) p(\vec{x}, t) = - \left[ \nabla \cdot \left( V(\vec{x}) + \nabla_{M(d\theta)}^{H^{-1}-I} D(\vec{x}) \right) \right] p(\vec{x}, t) + \frac{\beta t^{-\gamma}}{\Gamma(1-\gamma)} p_0(\vec{x}), \quad (1)$$

where  $b \geq 0$  and  $\beta \geq 0$  are arbitrary parameters,  $0 < \gamma < 1$  is the order of the Riemann-Liouville (R-L) fractional time derivative,  $p$  is a PDF,  $V$  is the velocity vector,  $D$  is the dispersion coefficient,  $p_0(x)$  denotes the initial condition,  $H^{-1}$  is the inverse of the scaling matrix providing the order and direction of the space fractional derivatives,  $I$  is the identity matrix, and  $M(d\theta)$  is the mixing measure.

The RWPT approximation of model (1) contains two components: jumping in space and waiting in immobile zones. The individual jump vector of each particle

at time step  $i$ , which is essentially a multiscaling compound Poisson process, can be calculated by [31]:

$$\vec{Z}(\tau) = \sum_{i=1}^{[\tau/d\tau]} \vec{x}_i = \sum_{i=1}^{[\tau/d\tau]} R_i^H \cdot \vec{\theta}_i, \quad (2)$$

where  $\vec{Z}(\tau)$  represents the particle location at operational time  $\tau$ ,  $[\tau/d\tau]$  is the number of random jumps by time  $\tau$  using the step size  $d\tau$ ,  $R_i$  is the random length of the  $i$ th jump with the jump direction  $\vec{\theta}_i$  drawn independently from the mixing measure  $M(d\theta)$  in Eq. (1). The matrix  $R^H$  is anisotropic to allow direction-dependent jump sizes. If the eigenvectors of  $H$  are orthogonal (representing perpendicular growth directions for particles), the random displacement along the  $k$ th eigenvector of  $H$  (with the jump length probabilities fall off as  $P(R^{1/\alpha_k} > r) \propto r^{-\alpha_k}$ ) can be calculated by:

$$R^{1/\alpha_k} = \left[ D(x_k) \left| \cos \frac{\pi\alpha_k}{2} \right| d\tau \right]^{1/\alpha_k} dL_{\alpha_k} + \left[ (\alpha_k - 1) \left| \cos \frac{\pi(\alpha_k - 1)}{2} \right| \right. \\ \left. \times d\tau \right]^{1/(\alpha_k - 1)} \Theta \left| \frac{\partial D}{\partial x_k} \right|^{1/(\alpha_k - 1)} dL_{\alpha_k - 1}, \quad (3)$$

where  $\Theta = 1, -1$ , and  $0$  if  $\partial D/\partial x_k > 0, < 0$ , and  $0$ , respectively;  $dL_{\alpha_k}$  and  $dL_{\alpha_k - 1}$  denote the  $\alpha_k$ - and  $\alpha_k - 1$ -order standard stable random variables with the maximum skewness, scale one, and zero shift.

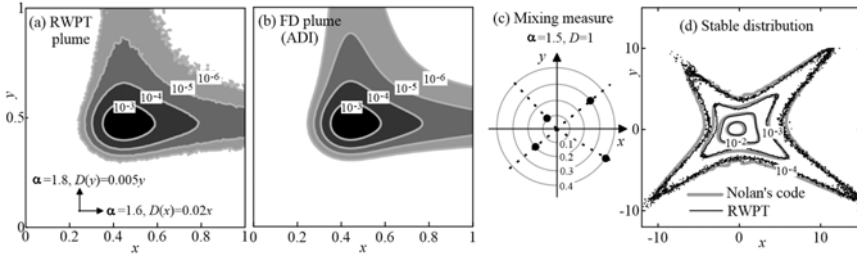
If the scaling matrix  $H$  contains nonorthogonal eigenvectors such as plume growing in a fractured aquifer with nonorthogonal fracture orientations, the mixing measure and the scaling matrix would have the same directions, and the jump vectors  $R^{1/\alpha_k}$  along each eigenvector are independent [32].

In the second step, the operational time can be simulated as the number of renewals by time  $T > 0$  for a given waiting time distribution with power-law probability tails:

$$dT = b d\tau + \left[ \beta \left| \cos \frac{\pi\gamma}{2} \right| d\tau \right]^{1/\gamma} dS_\gamma. \quad (4)$$

where  $dS_\gamma$  is a  $\gamma$ -order, standard stable random variable. Note here the particle motion is not instantaneous, and thus we can distinguish the status (mobile or immobile) for each particle at any given time. This distinction is critical in modeling field-measured plumes, since the sampling process tends to collect mobile solutes preferentially.

Numerical examples of the above RWPT are shown in Figure 1, where the Lagrangian solutions generally match the other numerical solutions. It is also noteworthy that the mixing measure and scaling matrix defined in the vector FADE (1) provides a convenient way to capture complex diffusion in a system with limited



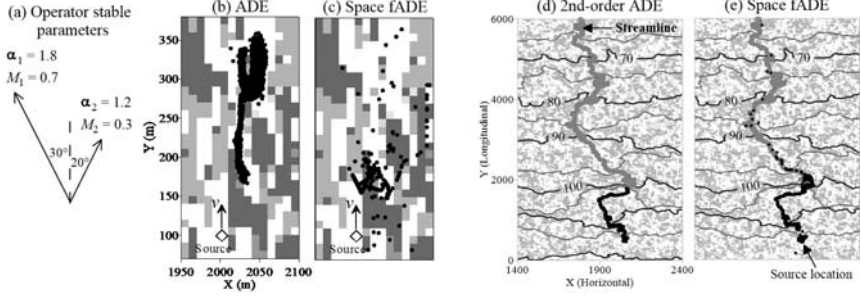
**Fig. 1:** Comparison of numerical solutions for the FADE (1). Case 1 (modified from [31]): the RWPT solution (a) vs. the implicit Euler finite difference solution (b) for the FADE (1) with orthogonal eigenvectors in the scaling matrix  $H$ . Case 2: Polar plot of the discrete mixing measure showing four directions and weights (c) and the RWPT solution vs. Nolan's [23] multivariate stable distribution (i.e.,  $H$  with nonorthogonal eigenvectors).

information in local velocities. This feature can be useful in hydrologic sciences, since many field sites have only limited subsurface information and can only provide a coarse resolution of the actual velocity field.

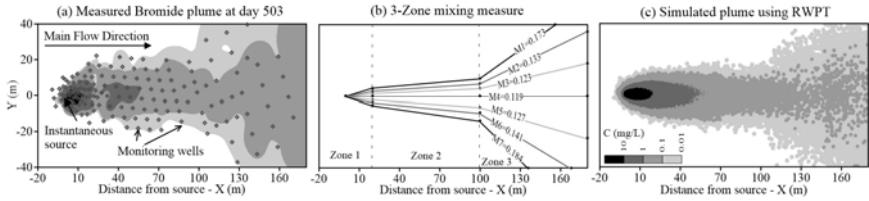
### 2.3 Vector FDE with space-dependent mixing measure

The above RWPT considers a constant mixing measure  $M(d\theta)$  in the FADE (1), while real-world diffusion may require a variable  $M(d\theta)$ . Mechanical dispersion in natural geological media represents the local variation of transport speed deviating from the mean velocity. The dispersion tensor in classical Fickian dispersion is usually aligned with the velocity vector, whose orientation may not remain constant but can change with the medium's internal architecture and/or external forcing. Generalizing to super-diffusion, the eigenvectors of the fractional derivative and the weights in the mixing measure will not be fixed in space, but may vary with streamlines. One example is the ancient, interconnected braided river channels (i.e., the direction of channels fluctuates in space) in alluvial deposits, which form the major preferential flow paths for super-diffusive solutes. The other example is the regional-scale fractured rock masses whose orientation can change in space due to the change of stress fields and tectonic dynamics. Both media can motivate super-diffusion with a space-dependent mixing measure.

Here we define a streamline-dependent mixing measure, with the mean flow advected along streamlines. The streamline projection approach proposed by Zhang et al. [31] can track the resultant particle motion. One example is shown in Figure 2. During each jump, we assign a random jump length  $L$ , and a random



**Fig. 2:** Particle plumes for the ADE (b) and the vector FADE (1) (c), given the streamline-dependent operator stable parameters defined in (a). The direction of  $V$  shows the mean flow direction. 10,000 particles were released at the point showing with a diamond. Plots (d) and (e) show the particle plumes of RWPT along streamlines, where the vector FADE (1) has parameters  $\alpha = 1.8$ ,  $\beta = 0$ , and time  $t = 5$ .

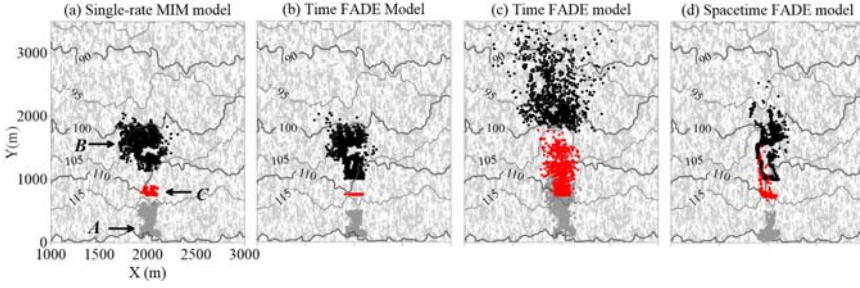


**Fig. 3:** Application of the FADE (1) with a variable mixing measure for the MADE site: the measured Bromide plume at day 503 (a), the best-fit three zone mixing measure with seven discrete directions and weights (b), and the RWPT plume (c) (modified from [32]).

direction  $\theta$  according to the local velocity vector and the local mixing measure. Then the particle's displacement  $L$  is projected to adjacent streamlines, along the angle  $\theta$ . The angle  $\theta$  is then adjusted to the new direction of  $v(x)$  and the particle is reprojected in the next jump. The FADE (1) with a variable mixing measure was found to capture the expanded, fan-shape plume observed at the well-known MADE test site, an alluvial aquifer in Mississippi (Figure 3) [32].

The above RWPT can be simplified if the mechanical dispersion is assumed to follow the stable distribution and particle super-diffusion follows exactly the streamlines. These two fundamental assumptions lead to the subordination to general flow model [2]:

$$\left( b \frac{\partial}{\partial t} + \beta \frac{\partial^y}{\partial t^y} \right) p = -\nabla \cdot \vec{v} p + \sigma^* (\nabla \cdot \vec{v})^\alpha p + \nabla [D^* \nabla p] + \frac{\beta t^{-y}}{\Gamma(1-y)} p_0(\vec{x}), \quad (5)$$



**Fig. 4:** Particle plumes for bimolecular reaction  $A + B \rightarrow C$  calculated by RWPT (snapshots at time  $t = 5$ ): Single-rate mobile-immobile transport model, with rate coefficient 1 and capacity coefficient 1 (a). Time FADE (5) with factor  $\sigma^* = 0$ , capacity coefficient  $\beta = 0.1$ , and the time index  $\gamma = 0.1$  (b) and 0.5 (c). The full FADE model (5) with the space index  $\alpha = 1.6$ ,  $\beta = 0.1$ , and  $\gamma = 0.1$  (d). Reactants  $A$  and  $B$  and the product  $C$  are represented by grey, black, and red particles, respectively.

where the advection operator  $\nabla_{\vec{v}}$  is defined via  $\nabla_{\vec{v}} = \nabla(\vec{V}p)$ ,  $\sigma^*$  is a scalar factor, and  $D^*$  is the molecular diffusivity. Model (5) shows that the density change is due to the advective flux  $\nabla_{\vec{v}}p$ , the subordinated mechanical dispersive flux  $\sigma^*(\nabla_{\vec{v}})^\alpha p$ , and the molecular diffusive flux  $\nabla[D^*\nabla p]$ . In saturated porous media, super-diffusion due to fast motion of dissolved chemicals along preferential flow paths does not deviate from  $v(x)$  (with a certain angle) but follow exactly the streamlines. This subordinated flow model improves the computational efficiency of the RWPT scheme, allowing additional processes (such as bimolecular reactions) to be added to particle tracking. One example is shown in Figure 4, where the Lagrangian solver calculates multi-scale reactive transport with small-scale chemical reactions and large-scale non-Fickian diffusion [34].

## 2.4 Bounded fractional diffusion

Natural processes are usually bounded, motivating the FDE and its Lagrangian solver in bounded domains. Zhang et al. [35] defined nonlocal boundary conditions and then developed a Lagrangian solver to approximate bounded, 1- $d$  fractional diffusion, which can be extended to multiple dimensions using the RWPT schemes reviewed above. Zhang et al. [35] showed that, to define Neumann and mixed Robin boundary conditions, the sign of R-L fractional derivative should remain consistent with the sign of the fractional-diffusive flux term in the FDE; otherwise the boundary value problem becomes ill-posed. Care is also required when approximating particle dynamics around the reflective boundary, where the exit-

ing particles can be either reflected (symmetrically) back to the internal domain for (local and symmetric) Fickian diffusion, or relocated at the boundary for (the nonlocal and nonsymmetric) fractional diffusion so that the reflected particles will not alter the overall dynamics of transport in the domain.

### 3 Future research directions

The low resolution in solution is one of the historical shortcomings for particle-based solvers. A large number of particles are required to reliably capture the large jump or long trapping for particles. To solve this issue, Allouch et al. (<https://arxiv.org/pdf/1707.03871.pdf>) developed particle-based, smooth particle approximations, which can obtain fine-resolution solutions for  $1-d$  space FDE with constant parameters. This approach, similar to smooth particle hydrodynamics, requires collections of particles to discretize the domain and therefore can be computational demanding. Another approach is to assign variable weights for particles located at different positions, and hence the resolution at low density regions may be improved without significant additional calculation.

RWPT algorithms for variable-order FDEs are also needed. Natural geological media can contain nonstationary heterogeneity, and water flow in aquifers and streams can change daily or seasonally, motivating the application of the FDEs with space and time dependent indexes. The corresponding Lagrangian solver has not been fully developed. In addition, natural processes can involve multi-scale dynamics, motivating the rapid development of multi-scale physical models. The multi-scale FDE and its Lagrangian solver remain to be shown.

### 4 Conclusion

We reviewed the fully Lagrangian solver to approximate the fractional differential equations. For the  $1-d$  FDE, both the Langevin approach and the fractional Lévy motion can define particle dynamics and guide the particle tracking schemes. For the vector FDEs with a constant mixing measure, the multiscaling compound Poisson process can be used to track particles moving along arbitrary directions with direction-dependent scaling rates. Real-world transport, however, may require a space-dependent mixing measure in the FDE, which can be modeled by the streamline projection and flow subordination methods in RWPT. Particle's trajectories affected by Dirichlet, Neumann, or mixed Robin boundary conditions can also be tracked using RWPT algorithms, leading to a fully Lagrangian approxima-



tion for the vector spatiotemporal FDEs with super-diffusion along streamlines in domains with any size and boundary conditions, as required by hydrological applications.

## A Langevin approach for 1- $d$ FDEs

We start with the forward equation, derive the backward equation by taking adjoints, and then apply the general theory of Markov processes [5] to obtain the Langevin equation. For example, the Langevin approach contains three steps to solve the following FDE:

$$\frac{\partial p(x, t)}{\partial t} = -\frac{\partial}{\partial x} [v(x) p(x, t)] + \frac{\partial^\alpha}{\partial x^\alpha} [D(x) p(x, t)] , \quad (6)$$

where  $1 < \alpha \leq 2$  is the order of R-L fractional space derivative. In step 1, using the fractional adjoint operator, one can derive the backward model of (6) [30]:

$$\frac{\partial p(x, t)}{\partial t} = v(x) \frac{\partial p(x, t)}{\partial x} + D(x) \frac{\partial^\alpha}{\partial (-x)^\alpha} p(x, t) . \quad (7)$$

Step 2 builds the Markov process, containing the backward generator  $Lu = v(x) \frac{\partial u}{\partial x} + \int [u(x+y) - u(x) - \frac{y}{1+y^2} \frac{\partial u(x)}{\partial x}] |\cos \frac{\pi\alpha}{2}| D(x) \phi(dy)$ , and the Langevin equation [5, 30]

$$dX(t) = v(X(t)) dt + \left[ D(X(t)) \left| \cos \frac{\pi\alpha}{2} \right| dt \right]^{1/\alpha} dL_\gamma . \quad (8)$$

The last step is to track particle dynamics defined by (8).

The Langevin approach can also solve the time FDE:

$$\left( b \frac{\partial}{\partial t} + \beta \frac{\partial^\gamma}{\partial t^\gamma} \right) p(x, t) = A_x p(x, t) + \beta \frac{t^{-\gamma}}{\Gamma(1-\gamma)} p_0(x) , \quad (9)$$

where  $A_x$  is the advection-diffusion operator such as that shown on the right-hand side of (6). Here we assume decoupled jump sizes and waiting times, and hence the density  $p$  in Eq. (9) can be calculated by subordinating the jump process against the waiting time process:

$$p(x, t) = \int_0^\infty u(x, \tau) h(\tau, t) d\tau , \quad (10)$$

where  $\tau$  denotes operational time. The first density  $u(x, \tau)$  in (10) models particle motion in  $\tau$ , which follows the Markov process (8) except that  $dt$  is replaced by  $d\tau$ . The second density  $h(\tau, t)$  accounts for the waiting times after each jump:

$$\frac{\partial}{\partial \tau} h(\tau, t) = - \left[ b \frac{\partial h(\tau, t)}{\partial t} + \beta \frac{\partial^\gamma h(\tau, t)}{\partial t^\gamma} \right] , \quad (11)$$

with initial condition  $h(\tau = 0, t) = b\delta(t) + \beta t^{-\gamma}/\Gamma(1 - \gamma)$ . Eq. (11) is analogous to (6), leading to the time Langevin equation (4) [32].

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