Stochastic solution of space-time fractional diffusion equations

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Classical and anomalous diffusion equations employ integer derivatives, fractional derivatives, and other pseudo-differential operators in space. In this paper we show that replacing the integer time derivative by a fractional derivative subordinates the original stochastic solution to an inverse stable subordinator process whose probability distributions are Mittag-Leffler. This leads to explicit solutions for space-time fractional diffusion equations with multiscaling space-fractional derivatives, and additional insight into the meaning of these equations.

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I. INTRODUCTION

Space-fractional diffusion equations [1–4] have been useful as models of anomalous transport in many diverse disciplines, including finance, semiconductor research, biology, and hydrogeology [5–7]. In the context of flow in porous media, fractional space derivatives model large motions through highly conductive layers or fractures, while fractional time derivatives describe particles that remain motionless for extended periods of time. Dissolved solutes may sorb to solid material [8] or diffuse into immobile-water zones of various sizes [9]. The scalar space-fractional diffusion equation governs Lévy motion, and the tail parameter α of the Lévy motion equals the order of the fractional derivative. Solutions to the vector space-fractional diffusion equation are operator Lévy motions [10] that may scale at different rates in different directions. The matrix exponent of the fractional derivative is related to the scaling rates in a similar manner [11, 12]. A more general diffusion equation governs any Lévy process $\boldsymbol{X}(t)$ [13, 14]. The probability density $p(\boldsymbol{x}, t)$ of any such process solves a diffusion-type equation

$$\frac{\partial p(\boldsymbol{x}, t)}{\partial t} = Lp(\boldsymbol{x}, t); \quad p(\boldsymbol{x}, 0) = \delta(\boldsymbol{x}), \tag{1}$$

where L is the generator of the Feller semigroup $S_t f(\boldsymbol{x}) = \int f(\boldsymbol{x} - \boldsymbol{y}) p(\boldsymbol{y}, t) d\boldsymbol{y}$ [15–17]. In this case, we say that $\boldsymbol{X}(t)$ is the stochastic solution to (1). The generator $Lf(\boldsymbol{x}) = \lim_{t \downarrow 0} t^{-1}(S_t f(\boldsymbol{x}) - f(\boldsymbol{x}))$. If $\boldsymbol{X}(t)$ is an α-stable Lévy motion without drift, then L is a fractional derivative operator of order α.

Fractional time derivatives are important in reactive transport, since solutes may interact with the immobile porous medium in highly nonlinear ways. There is evidence that solutes may sorb for random amounts of time that have a power law distribution [8], or move into irregularly-sized blocks of relatively immobile water, producing similar behavior [9]. If the first moment of these time delays diverges, then a fractional time derivative applies [6]. The fractional time derivative $\partial^\gamma g(t)/\partial t^\gamma$ for $0 < \gamma < 1$ is the inverse Laplace transform of $s^\gamma g(s)$, where $g(s) = \mathcal{L}[g(t)]$ is the usual Laplace transform. In this paper, we find the stochastic solution to the space-time fractional diffusion equation

$$\frac{\partial^\gamma q(\boldsymbol{x}, t)}{\partial t^\gamma} = Lq(\boldsymbol{x}, t) + \delta(\boldsymbol{x}) \frac{t^{-\gamma}}{\Gamma(1-\gamma)}. \tag{2}$$

We show that if $\boldsymbol{X}(t)$ is the stochastic solution to (1) then $\boldsymbol{X}(V_t)$ is the corresponding solution to (2), where V_t is the inverse Lévy process [18] for the stable subordinator with index γ. The fractional time derivative subordinates $\boldsymbol{X}(t)$ to the inverse stable subordinator V_t.

The space-time fractional diffusion equation is also connected with scaling limits of continuous time random walks (CTRW, see [6]). The spatial operator L depends on the jump size distribution [11, 12]. A fractional time derivative of order $0 < \gamma < 1$ pertains when the random waiting time T between jumps satisfies $P(T > t) \approx t^{-\gamma}$ so that $E(T) = \infty$. The infinite mean waiting time CTRW limit is the finite mean waiting time CTRW limit, subordinated to the inverse stable subordinator V_t.

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The random variable V_t has a Mittag-Leffler distribution [19] previously noted in connection with fractional time derivatives [4, 20] and relaxation [21].

II. CTRW SCALING LIMITS

CTRW were introduced [22, 23] to study random walks on a lattice. They are now used in physics to model a wide variety of phenomena connected with anomalous diffusion [23–25]. With finite mean waiting times, the jump process is asymptotically linear, and the CTRW behaves like the original random walk for large time [20, 26]. For a scalar process, finite variance jumps lead to Brownian motion in the scaling limit. Infinite variance jumps with power law tails lead to Lévy motion. Vector jumps with finite second moments lead to multivariable Brownian motion. Vector jumps with power law tails lead to multivariable Lévy motion, or operator Lévy motion if the power law behavior varies with the direction of motion [11, 12]. Speed of convergence to the CTRW scaling limit, and the implications for fractional diffusion modeling, are discussed in a recent paper of Barkai [27].

Many physical applications involve infinite mean waiting times [21, 28]. Introducing infinite mean waiting times has the effect of subordinating the CTRW scaling limit to the inverse process of a stable subordinator whose index γ is the same as the power law tail index of the waiting times. Essentially, this is because the counting process for particle jumps is inverse to the jump time process. The jump time process is asymptotically the stable subordinator, so the counting process for particle jumps is asymptotically the inverse stable subordinator.

A rigorous mathematical proof appears in [29]. We recount the basic ideas here to emphasize the physical applications. Given iid positive random variables J_i let $T_n = \sum_{i=1}^n J_i$ denote the time of the n-th particle jump. The position of the particle after the n-th jump is $\boldsymbol{W}(n) = \sum_{i=1}^n \boldsymbol{Y}_i$ where $\boldsymbol{Y}_i$ are iid and assumed independent of J_i. Then $N_t = \max\{n : T_n \le t\}$ counts the number of particle jumps by time $t > 0$ and the CTRW variable $\boldsymbol{W}(N_t)$ gives the position of the particle at time $t > 0$.

If $\boldsymbol{Y}$ has zero mean and finite second moments, the simple random walk of particle jumps

$$c^{-1/2}\boldsymbol{W}([ct]) \Rightarrow \boldsymbol{X}(t) \quad \text{as } c \to \infty \tag{3}$$

where the scaling limit $\boldsymbol{X}(t)$ is a Brownian motion. Shrinking the spatial coordinates by $c^{1/2}$ compensates expanding the time scale by c according to the central limit theorem. If $P(J > t) \approx t^{-\gamma}$ for some $0 < \gamma < 1$ then

$$c^{-1/\gamma}T_{[ct]} \Rightarrow B_t \quad \text{as } c \to \infty \tag{4}$$

according to the extended central limit theorem [15] where the scaling limit B_t is the stable subordinator process [13]. The γ-stable random variable B_t is totally positively skewed, hence this Lévy process is strictly increasing. The inverse process

$$V_\tau = \inf\{t : B_t > \tau\}$$

is also called the hitting time or first passage time process. Using the fact that T_n, N_t are inverse, so that $\{N_t \ge x\} = \{T_{\lceil x \rceil} \le t\}$, along with (4) yields

$$c^{-\gamma}N_{[ct]} \Rightarrow V_t \quad \text{as } c \to \infty.$$

Hence $N_{[ct]} \approx c^\gamma V_t$, and together with (3) this yields

$$c^{-\gamma/2}\boldsymbol{W}(N_{[ct]}) \approx (c^\gamma)^{-1/2}\boldsymbol{W}([c^\gamma V_t]) \Rightarrow \boldsymbol{X}(V_t)$$

as $c \to \infty$, so that the Brownian motion $\boldsymbol{X}(t)$ is subordinated to the inverse stable subordinator V_t.

The inverse processes have inverse distributional scaling $B_{ct} = c^{1/\gamma}B_t$ and $V_{ct} = c^\gamma V_t$, and together with the classical scaling for Brownian motion $\boldsymbol{X}(ct) = c^{1/2}\boldsymbol{X}(t)$ this shows that the CTRW limit is subdiffusive

$$\boldsymbol{X}(V_{ct}) = \boldsymbol{X}(c^\gamma V_t) = c^{\gamma/2}\boldsymbol{X}(V_t)$$

with Hurst index $H = \gamma/2 < 1/2$. Since $P(V_\tau \le t) = P(B_t \ge \tau) = P(t^{1/\gamma}B_1 \ge \tau) = P((B_1/\tau)^{-\gamma} \le t)$ the random variable V_τ has the same density function as $(\tau/B_1)^\gamma$. The density g_γ of the stable random variable B_1 has Laplace transform $\mathcal{L}[g_\gamma(t)] = e^{-s^\gamma}$. Computing moments of $(t/B_1)^\gamma$ shows that V_t has a Mittag-Leffler distribution [19]. If $p(\boldsymbol{x}, t)$ is the density of $\boldsymbol{X}(t)$ then a conditioning argument along with a simple change of variable shows that $\boldsymbol{X}(V_t)$ has density

$$\begin{aligned} q(\boldsymbol{x}, t) &= \int_0^\infty p(\boldsymbol{x}, (t/s)^\gamma) g_\gamma(s) ds \\ &= \frac{t}{\gamma}\int_0^\infty p(\boldsymbol{x}, u) g_\gamma(tu^{-1/\gamma}) u^{-1/\gamma - 1} du. \end{aligned} \tag{5}$$

Analytical estimates in [29] show that $q(\boldsymbol{k}, t) \ge C\|\boldsymbol{k}\|^{-b}$ for large $\|\boldsymbol{k}\|$, so $\boldsymbol{X}(V_t)$ does not have a normal density and hence cannot be a fractional Brownian motion [30].

If $P(\|\boldsymbol{Y}\| > r) \approx r^{-\alpha}$ for some $0 < \alpha < 2$ then $\boldsymbol{X}(t)$ is an α-stable Lévy motion and the CTRW limit $\boldsymbol{X}(V_t)$ has Hurst index $H = \gamma/\alpha$. If the tail index varies with the spatial coordinate, operator norming applies [12]. Then $\boldsymbol{X}(ct) = c^E\boldsymbol{X}(t)$ leads to $\boldsymbol{X}(V_{ct}) = c^{\gamma E}\boldsymbol{X}(t)$ so that the Hurst index $H = \gamma E$ is a matrix. For a diagonal exponent $E = \mathrm{diag}(1/\alpha_1, \ldots, 1/\alpha_d)$ the ith coordinate $X_i(t)$ is an α_i-stable Lévy motion and $X_i(V_t)$ is self-similar with Hurst index γ/α_i. Diagonalizable matrix exponents introduce a change of coordinates. Repeated eigenvalues thicken probability tails by a logarithmic factor, and complex exponents introduce rotations, leading to discrete scale invariance [31]. In every case, the scaling limit $\boldsymbol{X}(t)$ of the simple random walk is subordinated by the inverse stable subordinator V_t and the density changes from $p(\boldsymbol{x}, t)$ to $q(\boldsymbol{x}, t)$ via (5) when infinite mean waiting times are introduced. Next, we show that this change corresponds to a fractional time derivative in the diffusion equation.

III. TIME-FRACTIONAL DIFFUSION EQUATIONS

Wyss [32] and Schneider and Wyss [33] studied a time-fractional diffusion equation. Zaslavsky [34] introduced the space-time fractional kinetic equation (2) for Hamiltonian chaos. When $L = -v\partial/\partial x + D\partial^\alpha/\partial|x|^\alpha$ Saichev and Zaslavsky [35] show that if $p(\boldsymbol{x}, t)$ solves (1) then the function $q(\boldsymbol{x}, t)$ given by (5) solves (2). When $\alpha = 2$ they call the stochastic solution to (2) a "fractal Brownian motion." We prefer the term "time-fractional diffusion" to avoid confusing this process with the well-known fractional Brownian motion. In fact, if $\boldsymbol{X}(t)$ is a Brownian motion, the stochastic solution to (1) in this case, then the stochastic solution to (2) is $\boldsymbol{X}(V_t)$ where V_t is the inverse γ-stable subordinator. This interesting stochastic process is self-similar with Hurst index $\gamma/2$ so it is subdiffusive. However $\boldsymbol{X}(V_t)$ does not have a Gaussian distribution and it does not have stationary increments [29], so it is not fractional Brownian motion.

Barkai, Metzler, and Klafter [20] introduce a fractional Fokker-Planck equation equivalent to (2) with

$$L = -\frac{\partial}{\partial x}\frac{V'(x)}{m\eta_1} + K_1\frac{\partial^2}{\partial x^2}.$$

Barkai [4] applies (5), which he calls the inverse Lévy transform of $p(\boldsymbol{x}, t)$, to the solution of (1) in order to solve this fractional Fokker-Planck equation.

Scalar solutions to (1) with

$$L = -v\frac{\partial}{\partial x} + D\left(\frac{1-\beta}{2}\frac{\partial^\alpha}{\partial(-x)^\alpha} + \frac{1+\beta}{2}\frac{\partial^\alpha}{\partial x^\alpha}\right)$$

are α-stable densities [36, 37], purely symmetric when the skewness $\beta = 0$ [2, 38] and maximally skewed when $\beta = 1$ [3, 34]. When $\alpha = 2$ the skewness β is irrelevant, and the solutions are normal densities. Vector solutions for

$$L = -v \cdot \nabla + D\nabla^\alpha_m$$

are multivariable stable densities [11], where ∇^α_m is the operator with Fourier symbol

$$\int_{\|\theta\|=1} (ik \cdot \theta)^\alpha m(\theta) d\theta.$$

If $\alpha = 2$, this integral reduces to $(ik)A(ik)'$ where the matrix A has ij component $\int \theta_i\theta_j m(\theta)d\theta$, and solutions are vector Brownian motion.

Operator stable densities, where the stable index depends on the coordinate, solve (1) with

$$L = -v \cdot \nabla + \frac{1}{2}\nabla \cdot A\nabla + \mathcal{F}$$

where the generalized fractional derivative

$$\mathcal{F}f(x) = \int [f(x-y) - f(x) + y \cdot \nabla f(x)]\, d\phi(y)$$

and $d\phi(r^E\theta) = r^{-2}dr\, m(\theta)d\theta$ is an operator stable Lévy measure [10, 12, 39]. These are all abstract Cauchy problems [16, 17] whose solution $p(\boldsymbol{x}, t)$ is the family of densities for a Lévy process, a stationary independent increment process which includes Brownian motion and (operator) Lévy motion as special cases. Baeumer and Meerschaert [40] give a rigorous mathematical proof that any solution to the abstract Cauchy problem (1) is transformed to a solution of the fractional Cauchy problem (2) via the inverse Lévy transform (5). We summarize the essentials here in order to clarify the argument.

Use $s^{\gamma-1} = \mathcal{L}[t^{-\gamma}/\Gamma(1-\gamma)]$ and take Laplace-Fourier transforms ($\boldsymbol{x} \mapsto \boldsymbol{k}, t \mapsto s$) in (2) to get $s^\gamma q(\boldsymbol{k}, s) = \psi(\boldsymbol{k})q(\boldsymbol{k}, s) + s^{\gamma-1}$ where $\psi(\boldsymbol{k})$ is the Fourier symbol of L, so that $\mathcal{F}[Lf(x)] = \psi(\boldsymbol{k})f(\boldsymbol{k})$. Then

$$\begin{aligned} q(\boldsymbol{k}, s) &= \frac{s^{\gamma-1}}{s^\gamma - \psi(\boldsymbol{k})} \\ &= s^{\gamma-1}\int_0^\infty e^{-(s^\gamma - \psi(\boldsymbol{k}))u} du \\ &= \int_0^\infty s^{\gamma-1}e^{-s^\gamma u} p(\boldsymbol{k}, u) du \end{aligned} \tag{6}$$

using $\int_0^\infty e^{-au}du = a^{-1}$ and $p(\boldsymbol{k}, t) = e^{\psi(\boldsymbol{k})t}$, which follows from (1). Use $d(e^{-s^\gamma u})/ds = -\gamma s^{\gamma-1}ue^{-s^\gamma u}$ to get $s^{\gamma-1}e^{-s^\gamma u} = -(\gamma u)^{-1}d(e^{-s^\gamma u})/ds$. Recall that $e^{-s^\gamma} = \mathcal{L}[g_\gamma(t)]$ and write

$$\begin{aligned} e^{-s^\gamma u} &= e^{-(su^{1/\gamma})^\gamma} = \int_0^\infty e^{-su^{1/\gamma}v} g_\gamma(v) dv \\ &= \int_0^\infty e^{-st} g_\gamma(u^{-1/\gamma}t)u^{-1/\gamma} dt. \end{aligned}$$

Then compute

$$\begin{aligned} s^{\gamma-1}e^{-s^\gamma u} &= \frac{-1}{\gamma u}\frac{d}{ds}\left(\int_0^\infty e^{-st} g_\gamma(u^{-1/\gamma}t)u^{-1/\gamma} dt\right) \\ &= \frac{1}{\gamma u}\int_0^\infty te^{-st} g_\gamma(u^{-1/\gamma}t)u^{-1/\gamma} dt \end{aligned}$$

and combine with (6) to write $q(\boldsymbol{k}, s)$ as

$$\begin{aligned} &\int_0^\infty \left(\frac{1}{\gamma u}\int_0^\infty te^{-st} g_\gamma(u^{-1/\gamma}t)u^{-1/\gamma} dt\right) p(\boldsymbol{k}, u) du \\ &= \int_0^\infty e^{-st}\left(\int_0^\infty p(\boldsymbol{k}, u) g_\gamma(u^{-1/\gamma}t)\frac{t}{\gamma}u^{-1/\gamma-1} du\right) dt. \end{aligned}$$

Now invert the Laplace transform to obtain

$$q(\boldsymbol{k}, t) = \frac{t}{\gamma}\int_0^\infty p(\boldsymbol{k}, u) g_\gamma(tu^{-1/\gamma})u^{-1/\gamma-1} du$$

and invert the Fourier transform to get (5).

IV. CONCLUSIONS

Infinite mean waiting times subordinate CTRW scaling limits to an inverse stable subordinator, equivalent to applying an inverse Lévy transform (5) to the solution density. Since the solutions to time-fractional diffusion equations are also obtained via the inverse Lévy transform, a γ-fractional time derivative in a diffusion equation has the effect of subordinating the stochastic solution to the inverse process of a γ-stable subordinator. When applied to the classical diffusion equation, this procedure produces the "fractal Brownian motion" of Saichev and Zaslavsky as the solution to the time-fractional diffusion equation, a model for subdiffusion. This interesting stochastic process is not the same as fractional Brownian motion, but rather a completely new stochastic process. For CTRW models with coupled memory, in which particle jumps $\boldsymbol{Y}_i$ and waiting times J_i are dependent, the effect of infinite mean waiting times is more complicated [26]. In a forthcoming paper we will show that infinite mean waiting times in a coupled CTRW model also induce subordination by an inverse stable subordinator, but in that case the two processes are dependent.

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