Time Fractional Diffusion: A Discrete Random Walk Approach

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Abstract. The time fractional diffusion equation is obtained from the standard diffusion equation by replacing the first-order time derivative with a fractional derivative of order $\beta \in (0, 1)$. From a physical view-point this generalized diffusion equation is obtained from a fractional Fick law which describes transport processes with long memory. The fundamental solution for the Cauchy problem is interpreted as a probability density of a self-similar non-Markovian stochastic process related to a phenomenon of slow anomalous diffusion. By adopting a suitable finite-difference scheme of solution, we generate discrete models of random walk suitable for simulating random variables whose spatial probability density evolves in time according to this fractional diffusion equation.

Keywords: Anomalous diffusion, random walks, fractional derivatives, stochastic processes, self-similarity.

1. Introduction

Time and space fractional diffusion equations have been considered by several authors for different purposes. In particular, time fractional diffusion equations have been investigated by Mainardi (see, e.g., [1–3]) and by Metzler et al. (see, e.g., [4]) to show how the spatial variance of the fundamental solution is proportional to a fractional power of time, whereas space fractional diffusion equations have been investigated by Feller [5], West and Seshadri [6] and more recently by Gorenflo and Mainardi [7–9], see also [10, 11], to generate the class of Lévy stable probability densities. Time and space fractional diffusion equations have been jointly reviewed by Saichev and Zaslavsky [12], West et al. [13], and more recently by Anh and Leonenko [14], Gorenflo et al. [15, 16] and Mainardi et al. [17]. Random walk approaches to the fractional diffusion equations are usually derived from the Continuous-Time Random Walk Model (known simply as CTRW) that was formerly introduced and analyzed by Montroll and his associates (see, e.g., [18–20]. In this respect recent references include [12] and [21–29].

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The main physical purpose for adopting and investigating diffusion equations of fractional order is to describe phenomena of *anomalous diffusion* usually met in transport processes through complex and/or disordered systems including fractal media. In this respect an interesting review by Metzler and Klafter [30] has recently appeared to which (and references therein) we refer the interested reader. All the related models of random walk turn out to be beyond the classical Brownian motion, which is known to provide the microscopic foundation of the standard diffusion (see, e.g., [31]).

In this paper we intend to extend the approach by Gorenflo and Mainardi for the *space fractional diffusion* equation to the *time fractional diffusion* equation. This approach consists in proposing finite-difference schemes of solution that serve as discrete models of random walk. In the case of *space-fractional diffusion* these special random walks are related to *self-similar Markovian* stochastic processes which exhibit infinite space variance (*Lévy flights*) (see, e.g., [7–11]).

In Section 2, the fundamental solution of the *time fractional diffusion* equation is interpreted as a probability density of a *self-similar non-Markovian* stochastic process, which exhibits a space variance consistent with a phenomenon of *slow anomalous diffusion*. By adopting an appropriate finite-difference scheme of solution, we generate discrete models of random walk suitable for simulating random variables whose spatial probability density evolves in time according to this fractional diffusion equation. By properly scaled transition to vanishing space and time steps, these discrete models converge to the corresponding continuous processes.[1]

In Section 3, our finite-difference scheme is adopted in some case-studies for producing *sample paths* and the corresponding *space-increments* of individual particles performing the random walks. We have also computed *histograms* of the approximate realization of the corresponding probability densities by simulating many individual paths with the same number of time steps and making statistics of the final positions of the particles. Then, Section 4 is devoted to the conclusive discussions.

For possible convenience of the reader, we have reserved two Appendices for the notions of time fractional and space fractional derivatives that we use in this paper.

2. The Time Fractional Diffusion Equation

By *time fractional diffusion equation* we mean the evolution equation

$$ {}_tD_*^{\beta}\, u(x,t) = \frac{\partial^2}{\partial x^2}\, u(x,t), \quad 0 < \beta < 1, \quad x \in \mathbf{R}, \quad t \in \mathbf{R}_0^+, \tag{1}$$

where ${}_tD_*^{\beta}$ denotes the time fractional derivative intended in the *Caputo sense*, namely,

$$ {}_tD_*^{\beta}\, u(x,t) := \frac{1}{\Gamma(1-\beta)} \int_0^t \left[\frac{\partial}{\partial \tau}\, u(x,\tau)\right] \frac{\mathrm{d}\tau}{(t-\tau)^{\beta}}, \quad 0 < \beta < 1. \tag{2}$$

[1] This will be shown in a next paper.

For more details on the Caputo fractional derivative in the framework of the Riemann–Liouville fractional calculus we refer the interested reader to the Appendix A.[2] When $\beta = 1$ we recover in the limit the well-known diffusion equation,

$$\frac{\partial}{\partial t} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t), \quad x \in \mathbf{R}, \quad t \in \mathbf{R}_0^+. \tag{3}$$

In the above equations the use of proper non-dimensional variables is understood. Applying a time fractional integration of order β to both members of Equation (1) allows us to eliminate the time fractional derivative on the L.H.S.[3] leading to the alternative form of (1)

$$u(x,t) = u(x,0^+) + \frac{1}{\Gamma(\beta)} \int_0^t \left[\frac{\partial^2}{\partial x^2} u(x,\tau)\right] \frac{d\tau}{(t-\tau)^{1-\beta}}. \tag{4}$$

Differentiating (4) with respect to time we have another equivalent form

$$\frac{\partial}{\partial t} u(x,t) = \frac{1}{\Gamma(\beta)} \frac{\partial}{\partial t} \left\{ \int_0^t \left[\frac{\partial^2}{\partial x^2} u(x,\tau)\right] \frac{d\tau}{(t-\tau)^{1-\beta}} \right\}. \tag{5}$$

The Cauchy problem for the above evolution equations requires the knowledge of the initial condition $u(x,0^+) = f(x)$, where $f(x)$ denotes a given real function defined on $\mathbf{R}$, that we assume to be Fourier transformable in ordinary or generalized sense. We note that Equation (5) can be put in a *conservative form* as a *continuity equation*, namely

$$\frac{\partial}{\partial t} u(x,t) + \frac{\partial}{\partial x} F[u(x,t)] = 0, \tag{6}$$

where F is the *flux* given by

$$F[u(x,t)] = -\frac{\partial}{\partial x} \left\{ \frac{1}{\Gamma(\beta)} \frac{\partial}{\partial t} \left[\int_0^t u(x,\tau) \frac{d\tau}{(t-\tau)^{1-\beta}} \right] \right\}. \tag{7}$$

For $\beta = 1$ in (7) we recover in the limit the standard *Fick law*

$$F[u(x,t)] = -\frac{\partial}{\partial x} u(x,t), \tag{8}$$

which leads to the standard diffusion equation (3) by using the continuity law (6). We also note that Equation (7) can be interpreted as a generalized Fick law,[4] where (long) memory effects

[2] The most relevant formula is (41) which there calls to the game the initial value $f(0^+)$ corresponding here to the initial condition $u(x,0^+)$.

[3] From the definition of the Caputo fractional derivative (38) and from the semigroup property of the Riemann fractional integral (34) we note that

$$ {}_tJ^{\beta}\, {}_tD_*^{\beta}\, u(x,t) = {}_tJ^{\beta}\, {}_tJ^{1-\beta}\, {}_tD^1\, u(x,t) = {}_tJ^1\, {}_tD^1\, u(x,t) = u(x,t) - u(x,0^+).$$

[4] We recall that the Fick law is essentially a phenomenological law, which represents the simplest relationship between the flux F and the gradient of the concentration u. If u is a temperature, F is the heat-flux, so we speak of Fourier law. In both cases the law can be replaced by a more suitable phenomenological relationship which may account of possible non-local, non-linear and memory effects, without violating the conservation law expressed by the continuity equation.

are taken into account through a time fractional derivative of order $1-\beta$ in the *Riemann–Liouville* sense, see Appendix A.

Equations (1) and (3) can be seen as particular cases of the more general *space-time fractional diffusion* equation recently treated by Gorenflo et al. [15, 16] and Mainardi et al. [17],

$$ {}_tD_*^{\beta}\, u(x,t) = {}_xD_\theta^{\alpha}\, u(x,t), \quad x \in \mathbf{R}, \quad t \in \mathbf{R}^+, \tag{9}$$

where α, θ, β are real parameters restricted as follows

$$ 0 < \alpha \le 2, \quad |\theta| \le \min\{\alpha, 2-\alpha\}, \quad 0 < \beta \le 2. \tag{10}$$

In (9) ${}_tD_*^{\beta}$ is the Caputo time fractional derivative of order β, already defined (see also Appendix A) and ${}_xD_\theta^{\alpha}$ denotes the *Riesz–Feller* space fractional derivative of order α and skewness θ, which generalizes in a proper way the second order space-derivative as shown in Appendix B.

The fundamental solution or *Green function* of the space-time fractional diffusion equation (9) is intended to be the solution of the Cauchy problem corresponding to the initial condition $u(x,0^+) = \delta(x)$ when $0 < \beta \le 1$, or $u(x,0^+) = \delta(x)$, $u_t(x,0^+) = 0$ when $1 < \beta \le 2$. This solution, denoted by $G_{\alpha,\beta}^{\theta}(x,t)$, has been obtained in [17] by using the Mellin–Barnes integral representation. There it has been shown to be a *spatial probability density function* in the parameter ranges $\{0 < \alpha \le 2,\ 0 < \beta \le 1\}$ and $\{1 < \beta \le \alpha \le 2\}$, satisfying the *similarity law* for $t > 0$,

$$ G_{\alpha,\beta}^{\theta}(x,t) = t^{-\gamma}\, K_{\alpha,\beta}^{\theta}(x/t^{\gamma}), \quad \gamma = \beta/\alpha. \tag{11}$$

Here $K_{\alpha,\beta}^{\theta}(x) = G_{\alpha,\beta}^{\theta}(x,1)$ is called the reduced Green function. Note that $K_{\alpha,\beta}^{\theta}(-x) = K_{\alpha,\beta}^{-\theta}(x)$.

From the view-point of the discrete models of random walk related to Equation (9), only the cases with $\beta = 1$ (space-fractional diffusion) have been treated so far by our research group (see, e.g., [7–10]). There a Markovian description of Lévy flights has been obtained both for the symmetric ($\theta = 0$) and the asymmetric ($\theta \neq 0$) cases. Here we address our analysis to the cases of *time fractional diffusion* ($\alpha = 2, \theta = 0$) with the restriction $0 < \beta \le 1$.

Before providing the discrete random walk models related to the *time fractional diffusion* equation, its fundamental solution (corresponding to the initial condition $u(x,0^+) = \delta(x)$) is here recalled for the reader's convenience. Following the works by Mainardi [1–3], see also [17], the fundamental solution of our time fractional diffusion equation (1) turns out to be for $0 < \beta \le 1$

$$ G_{2,\beta}^{0}(x,t) = G_{2,\beta}^{0}(|x|,t) = \frac{1}{2\,t^{\beta/2}}\, M_{\beta/2}(r), \quad r = |x|/t^{\beta/2}, \tag{12}$$

where r acts as a *similarity variable*, and $M_{\beta/2}(r)$ is a transcendental function of Wright-type.[5] Being non-negative and normalized, such fundamental solution can be interpreted as a special

[5] For $0 < \nu < 1$ the function $M_\nu(z)$ ($z \in \mathbf{C}$) is entire of order $\rho = 1/(1-\nu)$. It can be defined by a power series or an integral over the Hankel path Ha:

$$ M_\nu(z) := \sum_{n=0}^{\infty} \frac{(-z)^n}{n!\,\Gamma[-\nu n + (1-\nu)]} = \frac{1}{2\pi i} \int_{\mathrm{Ha}} \mathrm{e}^{\sigma - z\sigma^{\nu}}\, \frac{\mathrm{d}\sigma}{\sigma^{1-\nu}}. $$

(space-symmetric) *pdf* whose main properties are herewith outlined. When $\beta = 1$ (standard diffusion) formula (12) reduces to the Gaussian *pdf* with variance $\sigma = 2t$, namely

$$G^0_{2,1}(x,t) = \frac{1}{2\sqrt{\pi}}\, t^{-1/2}\, \mathrm{e}^{-x^2/(4t)}. \tag{13}$$

From the exponential decay of the function $M_\nu(r)$ we can prove for $0 < \beta < 1$ the asymptotic representation as $|x| \to \infty$

$$G^0_{2,\beta}(|x|,t) \sim \frac{A(\beta)}{t^{\beta/2}} \left(\frac{x}{t^{\beta/2}}\right)^{q(\beta)} \exp\left[-B(\beta)\left(\frac{x}{t^{\beta/2}}\right)^{p(\beta)}\right], \tag{14}$$

where

$$\begin{cases} A = [2\pi(2-\beta)\, 2^{\beta/(2-\beta)} \beta^{(2-2\beta)/(2-\beta)}]^{-1/2}, \\ B = (2-\beta)\, 2^{-2/(2-\beta)} \beta^{\beta/(2-\beta)}, \end{cases} \tag{15}$$

$$\begin{cases} p = 2/(2-\beta), \\ q = (\beta-1)/(2-\beta). \end{cases} \tag{16}$$

Because of of (14–16) the moments of the *pdf* turn out to be

$$\int_{-\infty}^{+\infty} x^{2n}\, G^0_{2,\beta}(x,t)\, \mathrm{d}x = \frac{\Gamma(2n+1)}{\Gamma(\beta n+1)}\, t^{\beta n}, \quad n \in \mathbf{N}_0. \tag{17}$$

We recognize that the variance associated to the *pdf* is proportional to t^β, which for $0 < \beta < 1$ implies a phenomenon of *slow anomalous diffusion*. In the limiting case $\beta = 0$ we have

$$G^0_{2,0}(x,t) = \frac{1}{2}\, \mathrm{e}^{-|x|}, \tag{18}$$

meaning that the initial state $\delta(x)$ instantly freezes to a density decreasing exponentially in space but invariant in time.

3. The Discrete Non-Markovian Random Walk

We now sketch a *redistribution scheme* and a related discrete *random walk model* for our time fractional diffusion equation (1), including, in the limit for $\beta = 1$, the particular case of the standard diffusion (3), which leads to a discrete model of the classical Brownian motion. For this purpose we discretize space and time by grid points and time instants as follows

$$x_j = j\,h,\ h > 0,\ j = 0, \pm 1, \pm 2, \dots; \quad t_n = n\,\tau,\ \tau > 0, n = 0, 1, 2, \dots,$$

where the steps h and τ are assumed to be small enough. The dependent variable u is then discretized (after multiplication of (1) by the spatial mesh-width h) by introducing $y_j(t_n)$ as intended approximation to

$$\int_{x_j-h/2}^{x_j+h/2} u(x,t_n)\, \mathrm{d}x \approx h\, u(x_j, t_n). \tag{19}$$

With the quantities $y_j(t_n)$ so intended, we replace the time fractional diffusion equation (1), by the finite-difference equation

$$ {}_\tau D_*^\beta \, y_j(t_{n+1}) = \frac{y_{j+1}(t_n) - 2y_j(t_n) + y_{j-1}(t_n)}{h^2}, \quad 0 < \beta \le 1, \tag{20} $$

where the difference operator ${}_\tau D_*^\beta$ is intended to converge to ${}_t D_*^\beta$ as $\tau \to 0$. As usual, we have adopted a symmetric second-order difference quotient in space at level $t = t_n$ for approximating the second-order space derivative. For ${}_\tau D_*^\beta$ we require a form which must reduce as $\beta = 1$ to a forward difference quotient in time at level $t = t_n$, which is usually adopted for approximating the first-order time derivative, namely

$$ {}_\tau D_*^1 \, y_j(t_{n+1}) = \frac{y_j(t_{n+1}) - y_j(t_n)}{\tau}. \tag{21} $$

Then, for approximating the time fractional derivative (in Caputo's sense), we adopt a backward Grünwald–Letnikov scheme in time[6] (starting at level $t = t_{n+1}$) which reads

$$ {}_\tau D_*^\beta \, y_j(t_{n+1}) = \sum_{k=0}^{n+1} (-1)^k \binom{\beta}{k} \frac{y_j(t_{n+1-k}) - y_j(0)}{\tau^\beta}, \quad 0 < \beta \le 1. \tag{22} $$

Here the subtraction of $y_j(0)$ in each term of the sum reflects the subtraction of $f(0^+)$ in formula (41) for the Caputo fractional derivative. Combining (20) and (22), introducing the scaling parameter

$$ \mu := \frac{\tau^\beta}{h^2}, \quad 0 < \beta \le 1, \tag{23} $$

and using the 'empty sum' convention $\sum_{k=p}^{q} = 0$ if $q < p$ (here $p = 1$ when $q = n = 0$), we obtain for $n \ge 0$ ($t_0 = 0$):

$$ \begin{aligned} y_j(t_{n+1}) \; = \; & y_j(t_0) \sum_{k=0}^{n} (-1)^k \binom{\beta}{k} + \sum_{k=1}^{n} (-1)^{k+1} \binom{\beta}{k} y_j(t_{n+1-k}) \\ & + \mu [y_{j+1}(t_n) - 2y_j(t_n) + y_{j-1}(t_n)]. \end{aligned} \tag{24} $$

Thus, (24) provides the universal *transition law* from t_n to t_{n+1} valid for all $n \ge 0$. For convenience let us introduce the coefficients c_k, b_m

$$ \begin{cases} c_k = (-1)^{k+1} \binom{\beta}{k} = \left| \binom{\beta}{k} \right|, & k \ge 1, \\ b_m = \sum_{k=0}^{m} (-1)^k \binom{\beta}{k}, & m \ge 0. \end{cases} \tag{25} $$

For $\beta = 1$ (standard diffusion) we note that all these coefficients are vanishing except $b_0 = c_1 = 1$. For $0 < \beta < 1$ they possess the properties

$$ \sum_{k=1}^{\infty} c_k = 1, \quad 1 > \beta = c_1 > c_2 > c_3 > \ldots \to 0, \tag{26} $$

[6] Grünwald (1867) and Letnikov (1868) independently developed an approach to fractional differentiation for which the definition of the (Riemann–Liouville) fractional derivative is the limit of a fractional difference quotient (see, e.g., [32, 33]).

$$\begin{cases} b_0 = 1 = \sum_{k=1}^{\infty} c_k, \quad b_m = 1 - \sum_{k=1}^{m} c_k = \sum_{k=m+1}^{\infty} c_k, \\ 1 = b_0 > b_1 > b_2 > b_3 > \ \ldots \ \to 0. \end{cases} \tag{27}$$

We thus observe that the c_k and the b_m form sequences of positive numbers, not greater than 1, decreasing strictly monotonically to zero. Thanks to the introduction of the above coefficients the universal transition law (24) can be written in the following noteworthy form

$$y_j(t_{n+1}) = b_n \, y_j(t_0) + \sum_{k=1}^{n} c_k \, y_j(t_{n+1-k}) + \mu[y_{j+1}(t_n) - 2y_j(t_n) + y_{j-1}(t_n)], \tag{28}$$

with the empty sum convention if $n = 0$. In particular we get, for $n = 0$:

$$y_j(t_1) = (1 - 2\mu) \, y_j(t_0) + \mu \, [y_{j+1}(t_0) + y_{j-1}(t_0)];$$

for $n = 1$:

$$y_j(t_2) = b_1 y_j(t_0) + (c_1 - 2\mu) \, y_j(t_1) + \mu \, [y_{j+1}(t_1) + y_{j-1}(t_1)];$$

for $n \geq 2$:

$$\begin{aligned} y_j(t_{n+1}) \ &= \ b_n \, y_j(t_0) + \sum_{k=2}^{n} c_k \, y_j(t_{n+1-k}) \\ &\quad + (c_1 - 2\mu) \, y_j(t_n) + \mu[y_{j+1}(t_n) + y_{j-1}(t_n)]. \end{aligned}$$

Observe that $c_1 = \beta$. The scheme (28) *preserves non-negativity*, if all coefficients are non-negative, hence if

$$0 < \mu = \frac{\tau^{\beta}}{h^2} \leq \frac{\beta}{2}. \tag{29}$$

Furthermore it is *conservative*, as we shall prove by induction, i.e.,

$$\sum_{j=-\infty}^{+\infty} |y_j(t_0)| < \infty \implies \sum_{j=-\infty}^{+\infty} y_j(t_n) = \sum_{j=-\infty}^{+\infty} y_j(t_0), \quad n \in \mathbf{N}. \tag{30}$$

In fact, putting $S_n = \sum_{j=-\infty}^{+\infty} y_j(t_n)$ for $n \geq 0$, then from (28) we get

$$S_1 = (1 - 2\mu) \ \sum y_j(t_0) + \mu \sum y_{j-1}(t_0) + \mu \sum y_{j+1}(t_0) = S_0,$$

and for $n \geq 1$ we find always from (28), assuming $S_0 = S_1 = \ldots S_n$ already proved,

$$\begin{aligned} S_{n+1} \ &= \ b_n \, S_0 + \sum_{k=2}^{n} c_k \, S_{n+1-k} + (\beta - 2\mu + \mu + \mu) \, S_n \\ &= \ \left(b_n + \sum_{k=1}^{n} c_k \right) \, S_0 = S_0, \end{aligned}$$

using $\beta = c_1$. We have thus proved conservativity. Non-negativity preservation and conservativity mean that our scheme can be interpreted as a *redistribution scheme* of clumps

$y_j(t_n)$. For orientation on such aspects and for examples let us quote the works by Gorenflo on conservative difference schemes for diffusion problems (see, e.g., [34, 35]).

The interpretation of our *redistribution* scheme is as follows: the clump $y_j(t_{n+1})$ arises as a weighted-memory average of the (previous) $n+1$ values $y_j(t_m)$, with $m = n, n-1, \ldots, 1, 0$, with positive weights

$$\beta = c_1,\; c_2, \ldots, c_n, \quad b_n = 1 - \sum_{k=1}^{n} c_k, \tag{31}$$

followed by subtraction of $2\mu\, y_j(t_n)$, which is given in equal parts to the neighbouring points x_{j-1} and x_{j+1} but replaced by the contribution $\mu[y_{j+1}(t_n)+y_{j-1}(t_n)]$ from these neighbouring points. For *random walk* interpretation we consider the $y_j(t_n)$ as probabilities of sojourn at point x_j in instant t_n requiring the normalization condition $\sum_{j=-\infty}^{+\infty} y_j(t_0) = 1$.

For $n = 0$ Equation (28) means (by appropriate re-interpretation of the spatial index j): a particle sitting at x_j in instant t_0 jumps, when t proceeds from t_0 to t_1, with probability μ to the neighbour point x_{j+1}, with probability μ to the neighbour point x_{j-1}, and with probability $1-2\mu$ it remains at x_j. For $n \geq 1$ we write (28), using $\beta = c_1$, as follows:

$$\begin{aligned} y_j(t_{n+1}) \;=\; & \left(1 - \sum_{k=1}^{n} c_k\right) y_j(t_0) + c_n\, y_j(t_1) + c_{n-1}\, y_j(t_2) + \cdots + c_2\, y_j(t_{n-1}) \\ & + (c_1 - 2\mu)\, y_j(t_n) + \mu[y_{j+1}(t_n) + y_{j-1}(t_n)]. \end{aligned} \tag{32}$$

Obviously, all coefficients (probabilities) are non negative, and their sum is 1. But what does it mean? Having a particle, sitting in x_j at instant t_n, where will we find it with which probability at instant t_{n+1}? From (32) we conclude, by re-interpretation of the spatial index j, *considering the whole history* of the particle, i.e., the particle path $\{x(t_0),\; x(t_1),\; x(t_2),\; \ldots,\; x(t_n)\}$, that if at instant t_n it is in point x_j, there is the contribution $c_1 - 2\mu$ to be again at x_j at instant t_{n+1}, the contribution μ to go to x_{j-1}, the contribution μ to go to x_{j+1}. But the sum of these contributions is $c_1 = \beta \leq 1$. So, excluding the case $\beta = 1$ in which we recover the standard diffusion (*Markovian process*), for $\beta < 1$ we have to consider the previous time levels (*non-Markovian process*). Then, from level t_{n-1} we get the contribution c_2 for the probability of staying in x_j also at time t_{n+1}, from level t_{n-2} we get the contribution c_3 for the probability of staying in x_j at time $t_{n+1}, \ldots$, from level t_1 we get the contribution c_n for the probability of staying in x_j at time t_{n+1}, and finally, from level $t_0 = 0$ we get the contribution b_n for the probability of staying in x_j at time t_{n+1}. Thus, the whole history up to t_n decides probabilistically where the particle will be at instant t_{n+1}.

Let us consider the problem of *simulation* of transition from time level t_n to t_{n+1}: assume the particle sitting in x_j at instant t_n. Generate a random number equidistributed in $0 \leq \rho < 1$, and subdivide the interval [0, 1) as follows. From left to right beginning at zero we put adjacent intervals of length $c_1, c_2, \ldots, c_n, b_n$, for consistency left-closed, right-open. The sum of these is 1. We divide further the first interval (of length c_1) into sub-intervals of length $\mu, c_1 - 2\mu, \mu$. Then we look into which of the above intervals the random number falls. If in first interval with length $c_1 = \mu + (c_1 - 2\mu) + \mu$, then look in which subinterval, and correspondingly move the particle to x_{j-1}, or leave it at x_j or move to x_{j+1}. If the random number falls into one of the intervals with length $c_2,\; c_3,\; \ldots, c_n$ (i.e., c_k with $2 \leq k \leq n$), then move the particle back to its previous position $x(t_{n+1-k})$, which by chance could be identical with $x_j = x(t_n)$. If the random number falls into the rightmost interval with length b_n then move the particle

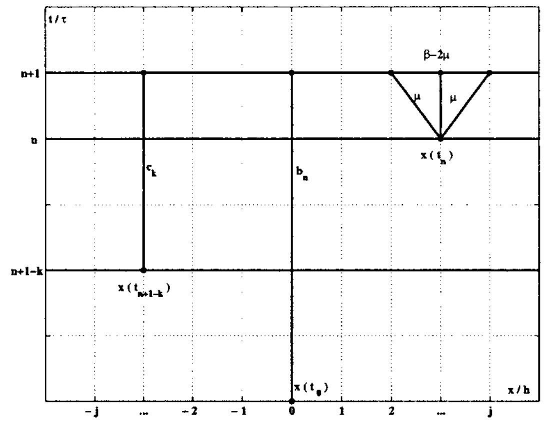

Figure 1. Sketch of the transition scheme for the random walker.

Table 1. β = fractional order, μ = scale parameter, h_S = space-step, τ_S = time-step for sample paths, h_H = space-step, τ_H = time-step for histograms.

β	$\mu < \beta/2$	h_S	τ_S	h_H	τ_H
1	0.4 < 1/2	0.07	2.0×10^{-3}	0.20	2.5×10^{-2}
0.75	0.3 < 3/8	0.17	2.0×10^{-3}	0.25	5.0×10^{-3}
0.50	0.2 < 1/4	0.47	2.0×10^{-3}	0.50	2.5×10^{-3}

back to its initial position $x(t_0)$, for which we recommend $x(t_0) = 0$, meaning $y_j(t_0) = \delta_{j0}$, in accordance with the initial condition $u(x, 0) = \delta(x)$ for (1). A sketch of the transition scheme for the random walker is reported in Figure 1. Besides the diffusive part (μ, $c_1 - 2\mu$, μ) which lets the particle jump at most to neighbouring points, we have for $0 < \beta < 1$ the memory part which gives a tendency to return to former positions even if they are far away. Due to Equations (26–27), of course, the probability to return to a far away point gets smaller and smaller the larger the time lapse is from the instant when the particle was there.

Herewith we present some results on the simulation of the sample paths (with increments apart) and histograms corresponding to some typical values of the index β, namely $\beta = 1$, 0.75, 0.50, in Figures 2, 3, 4, respectively. Our simulations are based on 10,000 realizations. The sample paths and the corresponding increments are plotted against the time steps up to 500 while the histograms refer to densities at $t = 1$ for $|x| \leq 5$. The relevant parameters μ, h and τ used in the figures are reported in Table 1.

4. Conclusions

Anomalous diffusion processes have in recent years gained revived interest among physicists, and methods of fractional calculus have shown their usefulness for purposes of modelling. In the time fractional case one is naturally led to a generalization of the classical diffusion equation with respect to the first-order time operator. One arrives in a natural way at non-Markovian processes in which space-probability distributions evolve in time consistently with the phenomenon of *slow anomalous diffusion* (with variance $\sigma^2 \propto t^\beta$, $0 < \beta < 1$).

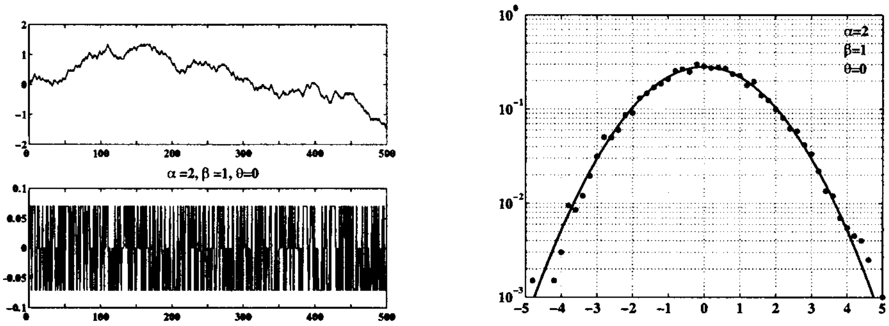

Figure 2. A sample path with increments (left), histogram (right) for $\beta = 1$.

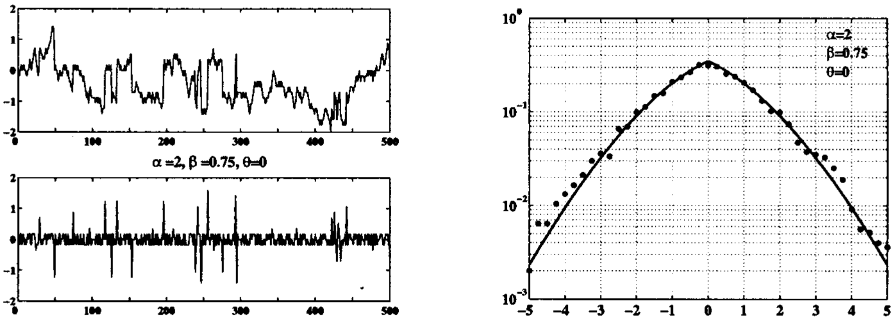

Figure 3. A sample path with increments (left), histogram (right) for $\beta = 0.75$.

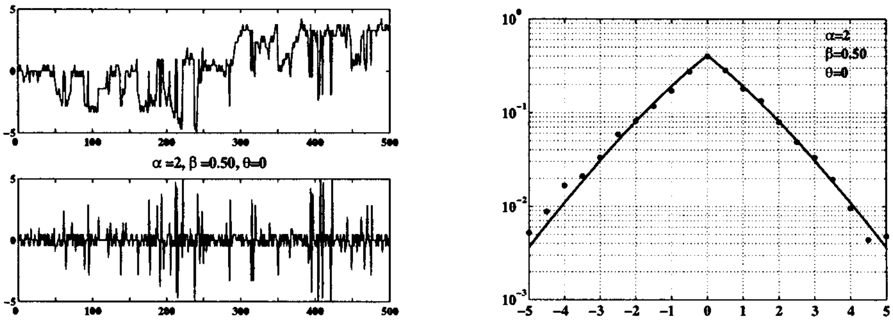

Figure 4. A sample path with increments (left), histogram (right) for $\beta = 0.50$.

In this paper we have provided a discrete random walk approach to this phenomenon. Let us stress the fact that our random walk model is obtained by discretizing the time fractional diffusion equation (1) in the most natural way. The difference scheme so obtained, with the scaling restriction (23), imitates on a discrete space-time grid the most essential properties of the continuous process, namely conservativity and preservation of non-negativity. Analogously, natural discretizations have likewise been successful in our papers [7–9] on rather general space fractional diffusion equations, and in a forthcoming paper we will demonstrate their use in general diffusion processes, fractional in space as well as in time [16].

Appendix A: The Riemann–Liouville and the Caputo Time Fractional Derivatives

For a sufficiently well-behaved function $f(t)$ $(t \in \mathbf{R}^+)$ we may define the fractional derivative of order β $(m-1 < \beta \le m, m \in \mathbf{N})$ (see, e.g., [32, 36]), in two different senses, that we refer here as to *Riemann–Liouville* derivative and *Caputo* derivative, respectively. Both derivatives are related to the so-called Riemann–Liouville fractional integral of order $\alpha > 0$ defined as

$$ {}_tJ^\alpha\, f(t) := \frac{1}{\Gamma(\alpha)} \int_0^t (t-\tau)^{\alpha-1}\, f(\tau)\, \mathrm{d}\tau, \quad \alpha > 0. \tag{33}$$

We recall the definition ${}_tJ^0 = I$ (Identity operator) and the semigroup property

$$ {}_tJ^\alpha\, {}_tJ^\beta = {}_tJ^\beta\, {}_tJ^\alpha = {}_tJ^{\alpha+\beta}, \quad \alpha, \beta \ge 0. \tag{34}$$

Furthermore

$$ {}_tJ^\alpha\, t^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1+\alpha)} t^{\gamma+\alpha}, \quad \alpha \ge 0, \quad \gamma > -1, \quad t > 0. \tag{35}$$

The fractional derivative of order $\beta > 0$ in the *Riemann–Liouville* sense is defined as the operator ${}_tD^\beta$ which is the left inverse of the Riemann–Liouville integral of order β, that is

$$ {}_tD^\beta\, {}_tJ^\beta = I, \quad \beta > 0. \tag{36}$$

If m denotes the positive integer such that $m-1 < \beta \le m$, we recognize from (34) and (36) ${}_tD^\beta\, f(t) := {}_tD^m\, {}_tJ^{m-\beta}\, f(t)$, hence

$$ {}_tD^\beta\, f(t) = \begin{cases} \dfrac{\mathrm{d}^m}{\mathrm{d}t^m} \left[\dfrac{1}{\Gamma(m-\beta)} \displaystyle\int_0^t \dfrac{f(\tau)\,\mathrm{d}\tau}{(t-\tau)^{\beta+1-m}} \right], & m-1 < \beta < m, \\ \dfrac{\mathrm{d}^m}{\mathrm{d}t^m} f(t), & \beta = m. \end{cases} \tag{37}$$

For completion we define ${}_tD^0 = I$.

On the other hand, the fractional derivative of order $\beta > 0$ in the *Caputo* sense is defined as the operator ${}_tD_*^\beta$ such that ${}_tD_*^\beta\, f(t) := {}_tJ^{m-\beta}\, {}_tD^m\, f(t)$, hence

$$ {}_tD_*^\beta\, f(t) = \begin{cases} \dfrac{1}{\Gamma(m-\beta)} \displaystyle\int_0^t \dfrac{f^{(m)}(\tau)\,\mathrm{d}\tau}{(t-\tau)^{\beta+1-m}}, & m-1 < \beta < m, \\ \dfrac{\mathrm{d}^m}{\mathrm{d}t^m} f(t), & \beta = m. \end{cases} \tag{38}$$

Thus, when the order is not inger the two fractional derivatives differ in that the derivative of order m does not generally commute with the fractional integral.

We point out that the *Caputo* fractional derivative satisfies the relevant property of being zero when applied to a constant, and, in general, to any power function of non-negative integer degree less than m, if its order β is such that $m-1 < \beta \le m$. Furthermore we note that (see, e.g., [32, 33]),

$$ {}_tD^\beta\, t^\gamma = \frac{\Gamma(\gamma+1)}{\Gamma(\gamma+1-\beta)}\, t^{\gamma-\beta}, \quad \beta \ge 0, \quad \gamma > -1, \quad t > 0. \tag{39}$$

Gorenflo and Mainardi [36] have shown the following relationships between the two fractional derivatives of the same non-integer order (when both of them exist),

$$
{}_tD_*^\beta f(t) = \begin{cases} {}_tD^\beta \left[f(t) - \sum_{k=0}^{m-1} f^{(k)}(0^+) \frac{t^k}{k!} \right], \\ {}_tD^\beta f(t) - \sum_{k=0}^{m-1} \frac{f^{(k)}(0^+)\, t^{k-\beta}}{\Gamma(k-\beta+1)}, \end{cases} \quad m-1 < \beta < m. \tag{40}
$$

In particular, if $m = 1$ we have

$$
{}_tD_*^\beta f(t) = \begin{cases} {}_tD^\beta \left[f(t) - f(0^+) \right], \\ {}_tD^\beta f(t) - \frac{f(0^+)\, t^{-\beta}}{\Gamma(1-\beta)}, \end{cases} \quad 0 < \beta < 1. \tag{41}
$$

The *Caputo* fractional derivative, practically ignored in the mathematical treatises, represents a sort of regularization in the time origin for the *Riemann–Liouville* fractional derivative. We note the different behaviour of the two fractional derivatives at the end points of the interval $(m-1, m)$ namely when the order is any positive integer, whereas ${}_tD^\beta$ is, with respect to its order β, an operator continuous at any positive integer, ${}_tD_*^\beta$ is an operator left-continuous since

$$
\lim_{\beta \to (m-1)^+} {}_tD_*^\beta f(t) = f^{(m-1)}(t) - f^{(m-1)}(0^+), \quad \lim_{\beta \to m^-} {}_tD_*^\beta f(t) = f^{(m)}(t).
$$

We also note for $m - 1 < \beta \le m$,

$$
{}_tD^\beta f(t) = {}_tD^\beta g(t) \Longleftrightarrow f(t) = g(t) + \sum_{j=1}^{m} c_j\, t^{\beta-j}, \tag{42}
$$

whereas,

$$
{}_tD_*^\beta f(t) = {}_tD_*^\beta g(t) \Longleftrightarrow f(t) = g(t) + \sum_{j=1}^{m} c_j\, t^{m-j}. \tag{43}
$$

In these formulae the coefficients c_j are arbitrary constants. Last but not least, we point out the major utility of the Caputo fractional derivative in treating initial-value problems for physical and engineering applications where initial conditions are usually expressed in terms of integer-order derivatives. This can be easily seen using the Laplace transformation, according to which

$$
\mathcal{L}\{{}_tD_*^\beta f(t); s\} = s^\beta \widetilde{f}(s) - \sum_{k=0}^{m-1} s^{\beta-1-k} f^{(k)}(0^+), \quad m-1 < \beta \le m, \tag{44}
$$

where

$$
\widetilde{f}(s) = \mathcal{L}\{f(t); s\} = \int_0^\infty \mathrm{e}^{-st} f(t)\, \mathrm{d}t, \quad s \in \mathbf{C}. \tag{45}
$$

We remind that the Laplace transform rule (44) was practically the starting point of Caputo himself in defining his generalized derivative (see, e.g., [37–39]).

5. Appendix B: The Riesz–Feller Space Fractional Derivative

For a sufficiently well-behaved function $f(x)$ whose Fourier transform is

$$\widehat{f}(\kappa) = \mathcal{F}\{f(x);\kappa\} = \int_{-\infty}^{+\infty} e^{+i\kappa x} f(x)\,dx, \quad \kappa \in \mathbf{R}, \tag{46}$$

we define the *Riesz–Feller* space fractional derivative of order α and skewness θ through

$$\mathcal{F}\left\{{}_xD_\theta^\alpha f(x);\kappa\right\} = -|\kappa|^\alpha e^{i(\mathrm{sign}\,\kappa)\theta\pi/2}\,\widehat{f}(\kappa), \tag{47}$$

where α and θ are restricted as in (10). Thus the *Riesz–Feller* derivative is the pseudo-differential operator[7] whose symbol is the logarithm of the characteristic function of a general *Lévy strictly stable* probability density with *index of stability* α and asymmetry parameter θ (improperly called *skewness*) according to Feller's parameterization [5, 33, 40], as revisited by Gorenflo and Mainardi in [7–9]. We note that for $\theta = 0$ the Riesz–Feller derivative can be interpreted as

$${}_xD_0^\alpha = -\left(-\frac{d^2}{dx^2}\right)^{\alpha/2}, \tag{48}$$

as can be formally deduced by writing $-|\kappa|^\alpha = -(\kappa^2)^{\alpha/2}$.

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[7] Let us recall that a generic linear pseudo-differential operator A, acting with respect to the variable $x \in \mathbf{R}$, is defined through its Fourier representation, namely

$$\int_{-\infty}^{+\infty} e^{i\kappa x} A[f(x)]\,dx = \widehat{A}(\kappa)\,\widehat{f}(\kappa),$$

where $\widehat{A}(\kappa)$ is referred to as symbol of A, given as $\widehat{A}(\kappa) = (A\,e^{-i\kappa x})\,e^{+i\kappa x}$.

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