Continuous time random walk and parametric subordination in fractional diffusion

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Abstract

The well-scaled transition to the diffusion limit in the framework of the theory of continuous-time random walk (CTRW) is presented starting from its representation as an infinite series that points out the subordinated character of the CTRW itself. We treat the CTRW as a combination of a random walk on the axis of physical time with a random walk in space, both walks happening in discrete operational time. In the continuum limit we obtain a (generally non-Markovian) diffusion process governed by a space-time fractional diffusion equation. The essential assumption is that the probabilities for waiting times and jump-widths behave asymptotically like powers with negative exponents related to the orders of the fractional derivatives. By what we call parametric subordination, applied to a combination of a Markov process with a positively oriented Lévy process, we generate and display sample paths for some special cases.

Keywords: Parametric subordination, random walks, anomalous diffusion, fractional calculus, renewal theory, power laws, Lévy processes.

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1 Introduction

Surveying the literature of the past 15 years we can observe an ever increasing interest in modelling anomalous diffusion processes, namely in diffusion processes deviating essentially from Gaussian behaviour which is characterized by evolution of the second centered moment like the first power of time. The reader interested to these processes is referred to several educational/review papers and books, including [2, 17, 18, 19, 21, 24, 31, 35, 36, 42, 43, 49, 55, 56, 59, 61, 63, 64].

In Section 2, we recall the simplest models for anomalous diffusion based on fractional calculus. They are obtained by replacing in the classical diffusion equation the partial derivatives with respect to space and/or time by derivatives of non-integer order, in such a way that the resulting Green function can still be interpreted as a probability density evolving in time differently from the Gaussian type.

A more general approach to anomalous diffusion is provided by the so-called continuous time random walk (CTRW) introduced in Statistical Mechanics by Montroll and Weiss [39], see also [37, 38, 40, 60], which differs from the usual models in that the steps of the walker occur at random times generated by a renewal process. The sojourn probability density of this process is known to be governed by an integral equation and expressed in terms of a relevant series expansion, as it will be recalled in Section 3. The concept of CTRW, can be understood by considering a random walk subordinated to a renewal process, see e.g. [9], as pointed out by a number of authors, see e.g. [1, 14, 26, 32, 50, 51, 52].

It is well known that the space-time fractional diffusion (STFD) equation and its variants, including the fractional Fokker-Planck equation, can be derived from the CTRW integral equation, see e.g. [4, 5, 20, 34, 35, 36, 42, 51, 53, 54], and references therein. More rigorously the passage from CTRW to STFD can be carried out via a properly scaled transition to the diffusion limit (under appropriate assumptions on waiting times and jumps), as shown in [58] and in a number of papers of our research group, see e.g. [12, 14, 15, 48].

In this paper, we offer another scheme of well-scaled transition to the diffusion limit, a scheme based on a modified concept of subordination that we call parametric subordination. To this purpose we lay open our general view of subordination in stochastic processes in Section 4. Then in Section 5, starting from the series expansion of the sojourn probability density in CTRW we arrive in a well-scaled limit process at the relevant integral formula for subordination.
Finally, we consider the problem of how to construct the sample paths for the STFD based on the above diffusion limit of the CTRW. In Section 6, we explain what we mean by parametric subordination whereas in Section 7, we describe the numerical procedure and provide sample paths for four case studies. The main conclusions are drawn in Section 8.

2 The space-time fractional diffusion

We begin by considering the Cauchy problem for the (spatially one-dimensional) space-time fractional diffusion equation

\[ t^\beta D_t^\beta u(x,t) = x^\theta D_\theta^\alpha u(x,t), \quad u(x,0) = \delta(x), \quad x \in \mathbb{R}, \quad t \geq 0, \tag{2.1} \]

where \( \{\alpha, \theta, \beta\} \) are real parameters restricted to the ranges

\[ 0 < \alpha \leq 2, \quad |\theta| \leq \min\{\alpha, 2 - \alpha\}, \quad 0 < \beta \leq 1. \tag{2.2} \]

Here \( t^\beta D_t^\beta \) denotes the Caputo fractional derivative of order \( \beta \), acting on the time variable \( t \), and \( x^\theta D_\theta^\alpha \) denotes the Riesz-Feller fractional derivative of order \( \alpha \) and skewness \( \theta \), acting on the space variable \( x \). Let us note that the solution \( u(x,t) \) of the Cauchy problem (2.1), known as the Green function or fundamental solution of the space-time fractional diffusion equation, is a probability density in the spatial variable \( x \), evolving in time \( t \). In the case \( \alpha = 2 \) and \( \beta = 1 \) we recover the standard diffusion equation for which the fundamental solution is the Gaussian density with variance \( \sigma^2 = 2t \).

Writing, with \( \Re[s] > \sigma_0, \kappa \in \mathbb{R} \), the transforms of Laplace and Fourier as

\[ \mathcal{L} \{ f(t); s \} = \tilde{f}(s) := \int_0^{\infty} e^{-st} f(t) \, dt, \]
\[ \mathcal{F} \{ g(x); \kappa \} = \tilde{g}(\kappa) := \int_{-\infty}^{+\infty} e^{i\kappa x} g(x) \, dx, \]

we have the corresponding transforms of \( t^\beta D_t^\beta f(t) \) and \( x^\theta D_\theta^\alpha g(x) \) as

\[ \mathcal{L} \{ t^\beta D_t^\beta f(t) \} = s^\beta \tilde{f}(s) - s^\beta - 1 f(0), \tag{2.3} \]
\[ \mathcal{F} \{ x^\theta D_\theta^\alpha g(x) \} = -|\kappa|^\alpha i^{\theta \text{sign} \kappa} \tilde{g}(\kappa). \tag{2.4} \]

Notice that \( i^{\theta \text{sign} \kappa} = \exp[i (\text{sign} \kappa) \theta \pi/2] \). For the mathematical details the interested reader is referred to [13, 25, 41] on the Caputo derivative, and to [44] on the Feller potentials. For the general theory of pseudo-differential
operators and related Markov processes the interested reader is referred to the excellent volumes by Jacob [22].

For our purposes let us here confine ourselves to recall the representation in the Laplace-Fourier domain of the (fundamental) solution of (2.1) as it results from the application of the transforms of Laplace and Fourier. Using \( \hat{\delta}(\kappa) \equiv 1 \) we have from (2.1)

\[
s^\beta \hat{u}(\kappa, s) - s^\beta - 1 = -|\kappa|^{\alpha} i \theta \text{sign } \kappa \hat{u}(\kappa, s),
\]

hence

\[
\hat{u}(\kappa, s) = \frac{s^\beta - 1}{s^\beta + |\kappa|^{\alpha} i \theta \text{sign } \kappa}.
\]

For explicit expressions and plots of the fundamental solution of (2.1) in the space-time domain we refer the reader to [27]. There, starting from the fact that the Fourier transform \( \hat{u}(\kappa, t) \) can be written as a Mittag-Leffler function with complex argument, the authors have derived a Mellin-Barnes integral representation of \( u(x,t) \) with which they have proved the non-negativity of the solution for values of the parameters \( \{\alpha, \theta, \beta\} \) in the range (2.2) and analyzed the evolution in time of its moments. In particular for \( \{0 < \alpha < 2, \beta = 1\} \) we obtain the stable densities of order \( \alpha \) and skewness \( \theta \).

The representation of \( u(x,t) \) in terms of Fox \( H \)-functions can be found in [29]. We note, however, that the solution of the STFD Equation (2.1) and its variants has been investigated by several authors as pointed out in the bibliography in [27]: here we refer to some of them, [1, 3, 33, 35], where the connection with the CTRW was also pointed out.

3 The continuous-time random walk

The name continuous time random walk (CTRW) became popular in physics after Montroll, Weiss and Scher (just to cite the pioneers) in the 1960s and 1970s published a celebrated series of papers on random walks for modelling diffusion processes on lattices, see e.g. [37, 39], and the book by Weiss [60] with references therein. CTRWs are rather good and general phenomenological models for diffusion, including processes of anomalous transport, that can be understood in the framework of the classical renewal theory, as stated e.g. in the booklet by Cox [9]. In fact a CTRW can be considered as a compound renewal process (a simple renewal process with reward) or a random walk subordinated to a simple renewal process.

Basic notions of the CTRW theory, that hereafter we briefly recall for the readers’ convenience, are the master equation (in integral form) for the
sojourn probability density, its Fourier-Laplace representation (known as the Montroll-Weiss formula) and its series representation.

A CTRW is generated by a sequence of independent identically distributed (i.i.d) positive random waiting times $T_1, T_2, T_3, \ldots$, each having the same probability density function $\phi(t)$, $t > 0$, and a sequence of i.i.d random jumps $X_1, X_2, X_3, \ldots$, in $\mathbb{R}$, each having the same probability density $w(x)$, $x \in \mathbb{R}$.

Let us remark that, for ease of language, we use the word density also for generalized functions in the sense of Gel’fand and Shilov [11], that can be interpreted as probability measures. Usually the probability density functions are abbreviated by pdf. We recall that $\phi(t) \geq 0$ with \[ \int_0^{\infty} \phi(t) \, dt = 1 \]

and $w(x) \geq 0$ with \[ \int_{-\infty}^{\infty} w(x) \, dx = 1. \]

Setting $t_0 = 0$, $t_n = T_1 + T_2 + \ldots T_n$ for $n \in \mathbb{N}$, the wandering particle makes a jump of length $X_n$ in instant $t_n$, so that its position is $x_0 = 0$ for $0 \leq t < T_1 = t_1$, and $x_n = X_1 + X_2 + \ldots X_n$, for $t_n \leq t < t_{n+1}$. We require the distribution of the waiting times and that of the jumps to be independent of each other. So, we have a compound renewal process (a renewal process with reward), compare [9].

By natural probabilistic arguments we arrive at the integral equation for the probability density $p(x, t)$ (a density with respect to the variable $x$) of the particle being in point $x$ at instant $t$, see e.g. [14, 16, 30, 46, 47, 48],

\[ p(x, t) = \delta(x) \Psi(t) + \int_0^t \phi(t - t') \left[ \int_{-\infty}^{\infty} w(x - x') p(x', t') \, dx' \right] \, dt', \quad (3.1) \]

in which the survival function

\[ \Psi(t) = \int_t^{\infty} \phi(t') \, dt' \quad (3.2) \]

denotes the probability that at instant $t$ the particle is still sitting in its starting position $x = 0$. Clearly, (3.1) satisfies the initial condition $p(x, 0) = \delta(x)$. In the Laplace-Fourier domain Eq. (3.1) reads as

\[ \hat{p}(\kappa, s) = \hat{\Psi}(s) + \hat{w}(\kappa) \hat{\phi}(s) \hat{p}(\kappa, s), \]

and using $\hat{\Psi}(s) = (1 - \hat{\phi}(s))/s$, explicitly

\[ \hat{p}(\kappa, s) = \frac{1 - \hat{\phi}(s)}{s} \frac{1}{1 - \hat{w}(\kappa) \hat{\phi}(s)}. \quad (3.3) \]

This Laplace-Fourier representation is known in physics as the the Montroll-Weiss equation, so named after the authors, see [39], who derive it in 1965.
as the basic equation for the CTRW. By inverting the transforms one can find the evolution \( p(x, t) \) of the sojourn density for time \( t \) running from zero to infinity. In fact, recalling that \(|\hat{w}(\kappa)| < 1 \) and \(|\tilde{\phi}(s)| < 1 \), if \( \kappa \neq 0 \) and \( s \neq 0 \), Eq. (3.3) becomes

\[
\tilde{p}(\kappa, s) = \Psi(s) \sum_{n=0}^{\infty} [\tilde{\phi}(s) \hat{w}(\kappa)]^n = \sum_{n=0}^{\infty} \tilde{v}_n(s) \hat{w}_n(\kappa), \quad (3.4)
\]

and we promptly obtain the series representation of the continuous time random walk, see e.g. [9] (Ch. 8, Eq. (4)) or [60] (Eq. (2.101)),

\[
p(x, t) = \sum_{n=0}^{\infty} v_n(t) w_n(x) = \Psi(t) \delta(x) + \sum_{n=1}^{\infty} v_n(t) w_n(x), \quad (3.5)
\]

where the functions \( v_n(t) \) and \( w_n(x) \) are obtained by repeated convolutions in time and in space, \( v_n(t) = (\Psi \ast \phi^n)(t) \), and \( w_n(x) = (w^n)(x) \), respectively. In particular, \( v_0(t) = (\Psi \ast \delta)(t) = \Psi(t) \), \( v_1(t) = (\Psi \ast \phi)(t) \), \( w_0(x) = \delta(x) \), \( w_1(x) = w(x) \). In the R.H.S of Eq (3.5) we have isolated the first singular term related to the initial condition \( p(x, 0) = \Psi(0) \delta(x) = \delta(x) \). The representation (3.5) can be found without detour over (3.1) by direct probabilistic reasoning and transparently exhibits the CTRW as a subordination of a random walk to a renewal process: it can be used as starting point to derive the Montroll-Weiss equation, as it was originally recognized by Montroll and Weiss [39]. Though (3.5), while being an attractive general formula, is unlikely to lead to explicit answers to rather simple problems, we consider it as a basic and useful formula for our analysis, as it will be shown later on.

A special case of the integral equation (3.1) is obtained for the compound Poisson process where \( \phi(t) = m e^{-mt} \) (with some positive constant \( m \)). Then, the corresponding master equation reduces after some manipulations, that best are carried out in the Laplace-Fourier domain, to the Kolmogorov-Feller equation:

\[
\frac{\partial}{\partial t} p(x, t) = -m p(x, t) + m \int_{-\infty}^{+\infty} w(x - x') p(x', t) dx'. \quad (3.6)
\]

Then, the solution obtained via the series representation reads

\[
p(x, t) = \sum_{k=0}^{\infty} \frac{(mt)^k}{k!} e^{-mt} w_k(x). \quad (3.7)
\]

Note that only in this case the corresponding stochastic process is Markovian.
4 Subordination in stochastic processes

In recent years a number of papers have appeared where explicitly or implicitly subordinated stochastic processes have been treated in view of their relevance in physical and financial applications, see e.g. [11 41 46 32 35 48 50 51 52 57 59 62] and references therein. Historically, the notion of subordination was originated by Bochner, see [7 8].

We obtain the process \( X(t) \) of our proper interest in the form \( X(t) = Y(T_*(t)) \) by randomizing the time clock of a stochastic process \( Y(t) \) using a new clock \( t = T(t_*) \), the non-decreasing right-continuous random functions \( t = T(t_*) \) and \( t_* = T_*(t) \) being inverse (in the appropriate sense) to each other. The resulting process \( x = X(t) \) is said to be subordinated to the so-called parent process \( Y(t_*) \), and \( t_* \) is commonly referred to as the operational time.

Our essential process for randomizing time is the process \( t = T(t_*) \), called by us the leading process. Our view is in contrast to that of Bochner’s subordination adopted by Feller [10] and others, see e.g. [32 57], who put into the foreground the inverse process \( t_* = T_*(t) \), which actually is a hitting time or first passage process, and after Feller often called the directing process.

In particular, assuming \( Y(t_*) \) to be a Markov process with a spatial probability density function (pdf) of \( x \), evolving in operation time \( t_* \), \( q_{t_*}(x) \equiv q(x, t_*) \), and \( T_*(t) \) to be a process with non-negative, not necessarily independent, increments with pdf of \( t_* \) depending on a parameter \( t, r_t(t_*) \equiv r(t_*, t) \), then the subordinated process \( X(t) = Y(T_*(t)) \) is governed by the spatial pdf of \( x \) evolving with \( t, p_t(x) \equiv p(x, t) \), given by the integral formula of subordination (compare with Eq (7.1), Ch. X in [10] and with Eq. (3.1) in [28])

\[
p_t(x) = \int_0^\infty q_{t_*}(x) r_t(t_*) \, dt_* . \tag{4.1}
\]

If the parent process \( Y(t_*) \) is self-similar of the kind that its pdf \( q_{t_*}(x) \) is such that, with a probability density \( q(x) \) and a positive number \( \gamma \),

\[
q_{t_*}(x) \equiv q(x, t_*) = t_*^{-\gamma} q \left( \frac{x}{t_*^{\gamma}} \right) , \tag{4.2}
\]

then Eq. (4.1) reads

\[
p_t(x) = \int_0^\infty q \left( \frac{x}{t_*^{\gamma}} \right) r_t(t_*) \frac{dt_*}{t_*^{\gamma}} . \tag{4.3}
\]
Remark: Feller [10] and several other mathematicians, e.g. [22] [45], in their treatment of subordination, are mainly interested in Markov processes. After explicitly saying (in his Section X.7) that the subordinated process may happen to be non-Markovian, Feller immediately turns his attention to the search for conditions to be imposed on the directing process that ensure the subordinated process to be Markovian like the parent process. For our processes (see next Section) these conditions are in general not fulfilled.

5 Subordination in continuous time random walk

In fractional diffusion an intuitive understanding can be gained by formalizing the transition from the series representations (3.4) and (3.5) of a general continuous time random walk (CTRW), known in the mathematical literature as a renewal process with reward. We cannot survey the rich literature on the subject, but let us call here the reader’s special attention to the most recent papers by Piryatinska, Saichev and Woyczynski [42] and Sokolov and Klafter [54]. These authors show in differing ways how fractional diffusion can be obtained from continuous time random walk. In contrast to these authors we lay out in all details our method of well-scaled transition to the diffusion limit, making explicit the meaning of long-time wide-space behaviour. For the general principle of well-scaledness we refer to [12, 14, 15, 48].

In the series representation (3.5) for the CTRW the running index \( n \) corresponds to the so-called ”operational time” \( t_* \) in the subordination formula for a continuous (stable) process. We will pass in (3.5) to the diffusion limit under the ”power law” assumptions (in the Laplace-Fourier domain)

\[
1 - \tilde{\phi}(s) \sim \lambda s^\beta, \quad \lambda > 0, \quad s \to 0^+,
\]

\[
1 - \tilde{w}(\kappa) \sim \mu |\kappa|^\alpha \exp(i \theta \text{sign} \kappa), \quad \mu > 0, \quad \kappa \to 0,
\]

where \( \beta, \alpha \) and \( \theta \) are restricted as in (2.2). If \( 0 < \beta < 1 \) and \( 0 < \alpha < 2 \), Eqs. (5.1) and (5.2) imply fat (power-law) tails for the densities \( \phi(t) \) and \( w(x) \); otherwise, for \( \beta = 1 \), Eq. (5.1) implies that \( \phi(t) \) has a finite first moment (e.g. the exponential pdf), and, for \( \alpha = 2 \), Eq. (5.2) implies that \( w(x) \) has a finite second moment (e.g. the Gaussian pdf). For details we refer e.g. to [15].

The idea is to treat the series expansion (starting from \( n = 0 \)) in (3.5) as an approximation to an improper Riemann integral. Being interested on behaviour in large time and wide space we change the units of measurement in order to make large time intervals and space distances appear numerically
of moderate size, moderate time intervals and space distances of small size. To this aim we replace waiting times $T$ by $\tau T$, jumps $X$ by $hX$, and then send the positive scaling factors $\tau$ and $h$ to zero, observing a scaling relation that will become mandatory in our calculations. For conciseness of our presentation we skip the analytical subtleties of interchanges of summations and integrations. For a strictly analytical derivation of our final integral equation of subordination we recommend \[28\].

For the CTRW this means replacing $\phi(t)$ by $\widetilde{\phi}(t/\tau) = \phi(t/\tau)$, $w(x)$ by $w_h(x) = w(x/h)/h$, correspondingly $\phi(s)$ by $\widetilde{\phi}(s) = \phi(s)$, $\bar{w}(\kappa)$ by $\bar{w}_h(\kappa) = \bar{w}(h\kappa)$. Decorating (3.5) by indices $h$ and $\tau$ gives

$$p_{h,\tau}(x, t) = \sum_{n=0}^{\infty} v_{\tau,n}(t) w_{h,n}(x), \quad (5.3)$$

yielding in the Fourier-Laplace domain

$$\widehat{p}_{h,\tau}(\kappa, s) = \sum_{n=0}^{\infty} \frac{1 - \widetilde{\phi}(\tau s)}{s} \left( \widetilde{\phi}(\tau s) \right)^n \left( \widehat{w}(h\kappa) \right)^n. \quad (5.4)$$

Separately we treat the powers $\left( \widetilde{\phi}(\tau s) \right)^n$ and $\left( \widehat{w}(h\kappa) \right)^n$, so avoiding the problematic simultaneous inversion of the diffusion limit from the Fourier-Laplace domain into the physical domain.

Observing from (5.1)

$$\left( \widetilde{\phi}(\tau s) \right)^n \sim \left( 1 - \lambda(\tau s)^\beta \right)^n, \quad (5.5)$$

we relate the running index $n$ to the presumed operational time $t_*$ by

$$n \sim \frac{t_*}{\lambda \tau \beta}, \quad (5.6)$$

and for fixed $s$ (as required by the continuity theorem of probability theory), by sending $\tau \to 0$ we get

$$\left( \widetilde{\phi}(\tau s) \right)^n \sim \left( 1 - \lambda \tau^\beta s^\beta \right)^{t_*/(\lambda \tau^{\beta})} \to \exp \left( -t_* s^\beta \right). \quad (5.7)$$

Here $s$ corresponds to physical time $t$, and in Laplace inversion we must treat $t_*$ as a parameter. Hence, in physical time $\exp(-t_* s^\beta)$ corresponds to

$$\bar{g}_\beta(t, t_*) = t_*^{-1/\beta} \bar{g}_\beta(t_*^{-1/\beta} t), \quad (5.8)$$
with \( \bar{g}_\beta(s) = \exp(-s^\beta) \). Here \( \bar{g}_\beta(t,t_*) \) is the totally positively skewed stable density (with respect to the variable \( t \)) evolving in operational time \( t_* \) according to the "space"-fractional equation

\[
\frac{\partial}{\partial t_*} \bar{g}_\beta(t,t_*) = t D_{-\beta} \bar{g}_\beta(t,t_*) , \quad \bar{g}_\beta(t,0) = \delta(t) ,
\]  

(5.9)

where \( t \) is playing the role of the spatial variable. Analogously, observing from (5.2)

\[
(\hat{w}(h\kappa))^n \sim \left(1 - \mu(h|\kappa|)^\alpha s^{\theta \text{sign} \kappa}\right)^n,
\]  

(5.10)

and with the aim of obtaining a meaningful limit we now set

\[
n \sim \frac{t_*}{\mu h^\alpha},
\]  

(5.11)

and find, by sending \( h \to 0^+ \), the relation

\[
(\hat{w}(h\kappa))^n \sim \left(1 - \mu(h|\kappa|)^\alpha s^{\theta \text{sign} \kappa}\right)^{t_*/(\mu h^\alpha)} \to \exp\left(-t_*|\kappa|^\alpha s^{\theta \text{sign} \kappa}\right),
\]  

(5.12)

the Fourier transform of a \( \theta \)-skewed \( \alpha \)-stable density \( f_{\alpha,\theta}(x,t_*) \) evolving in operational time \( t_* \). This density is the solution of the space-fractional equation

\[
\frac{\partial}{\partial t_*} f_{\alpha,\theta}(x,t_*) = x D_{\theta} f_{\alpha,\theta}(x,t_*) , \quad f_{\alpha,\theta}(x,0) = \delta(x) .
\]  

(5.13)

The two relations (5.6) and (5.11) between the running index \( n \) and the presumed operational time \( t_* \) require the (asymptotic) scaling relation

\[
\lambda t^\beta \sim \mu h^\alpha ,
\]  

(5.14)

that for purpose of computation we simplify to

\[
\lambda t^\beta = \mu h^\alpha .
\]  

(5.15)

Replacing \( t_* \) by \( t_{*n} = n \lambda t^\beta \), using the asymptotic results (5.7) and (5.12) obtained for the powers \( \left(\bar{\phi}(\tau s)\right)^n \) and \( (\hat{w}(h\kappa))^n \), furthermore noting

\[
\frac{1 - \bar{\phi}(\tau s)}{s} \sim s^{\beta-1} \lambda t^\beta ,
\]  

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we finally obtain from (5.4) the Riemann sum (with increment $\lambda \tau^\beta$)
\[
\hat{p}_{h,\tau}(\kappa, s) \sim s^{\beta - 1} \sum_{n=0}^{\infty} \exp \left[ -n\lambda \tau^\beta \left(s^\beta + |\kappa|^\alpha_i \theta \text{sign } \kappa \right) \right] \lambda \tau^\beta,
\]
and hence the integral
\[
\hat{p}_{h,\tau}(\kappa, s) \sim s^{\beta - 1} \int_{0}^{\infty} \exp \left[ -t\tau^\beta \left(s^\beta + |\kappa|^\alpha_i \theta \text{sign } \kappa \right) \right] dt.
\]
For the limiting process $u_\beta(x, t)$ this means
\[
\hat{u}_\beta(\kappa, s) = \int_{0}^{\infty} s^{\beta - 1} \exp \left[ -t\tau^\beta \left(s^\beta + |\kappa|^\alpha_i \theta \text{sign } \kappa \right) \right] dt.
\]
Observe that the RHS of this equation is just another way of writing the RHS of equation (2.5) which is the Laplace-Fourier solution of the STFD equation (2.1). By inverting the transforms we get after some manipulations (compare [32]) in physical space-time the integral formula of subordination
\[
u_\beta(x, t) = \int_{0}^{\infty} f_{\alpha, \theta}(x, t_*) g_\beta(t_*, t) dt_*
\]
with
\[
g_\beta(t_*, t) = t^{\beta - 1/\beta} g_{\beta} \left( t_*^{-1/\beta} \right) t_*^{-1/\beta - 1}
\]
standing for the density $r_t(t_*)$ in equation (4.1).

There are two processes involved. One is the unidirectional motion along the $t_*$ axis representing the operational time. This motion happens in physical time $t$ and the pdf for the operational time having value $t_*$ is (as density in $t_*$, evolving in physical time $t$) given by (5.20). In fact, by substituting $y = t t_*^{-1/\beta}$ we find
\[
\int_{0}^{\infty} g_\beta(t_*, t) dt_* \equiv \int_{0}^{\infty} \tilde{g}_\beta(t, t_*) dt = 1, \quad \forall t > 0.
\]
The operational time $t_*$ stands in analogy to the counting index $n$ in Eqs. (3.5) and (5.4). The other process is the process described by Eq. (5.13), a spatial probability density for sojourn of the particle in point $x$ evolving in operational time $t_*$,
\[
u_\beta(x, t_*) = f_{\alpha, \theta}(x, t_*).
\]
We get the solution to the Cauchy problem (2.1), namely the pdf $u(x, t) = u_\beta(x, t)$ for sojourn in point $x$, evolving in physical time $t$, by averaging $\bar{u}_\beta(x, t_*)$ with the weight function $g_\beta(t_*, t)$ over the interval $0 < t_* < \infty$ according to (5.19).
6 Sample path for space-time fractional diffusion

In the series representation (3.5) of the CTRW the running index \( n \) (the number of jumps having occurred up to physical time \( t \)) is a discrete operational time, proceeding in unit steps. To this index \( n \) corresponds the physical time \( t = t_n \), the sum of the first \( n \) waiting times, and in physical space the position \( x = x_n \), the sum of the first \( n \) jumps, see Section 3.

Rescaling space and physical time by factor \( h \) and \( \tau \), obeying the scaling relation

\[ \mu h^\alpha = \lambda \tau^\beta, \]  

(6.1)

and introducing, by sending \( \{h \to 0, \tau \to 0\} \), continuous operational time

\[ t_* \sim n \lambda \tau^\beta \sim n \mu h^\alpha. \]  

(6.2)

Then, in the series representation (3.5) we have two discrete Markov processes (discrete in operation time \( n \)), namely a random walk in the space variable \( x \), with jumps \( X_n \), and another random walk (only in positive direction) of the physical time \( t \), making a forward jump \( T_n \) at every instant \( n \).

In the diffusion limit the spatial process becomes an \( \alpha \)-stable process for the position \( \bar{x} = \bar{x}(t_*) \), whereas the unilateral time process becomes a unilateral (positively directed) \( \beta \)-stable process for the physical time \( t = \bar{t} = \bar{t}(t_*) \). A sample path of a diffusing particle in physical coordinates can be produced by combining in the \((t, x)\) plane the two random functions

\[ \begin{cases} x = \bar{x} = \bar{x}(t_*), \\ t = \bar{t} = \bar{t}(t_*), \end{cases} \]  

(6.3)

both evolving in operational time \( t_* \), both being Markovian and obeying stochastic differential equations

\[ \begin{cases} d\bar{x} = d(\text{Lévy noise of order } \alpha \text{ and skewness } \theta), \\ d\bar{t} = d(\text{one sided Lévy noise of order } \beta). \end{cases} \]  

(6.4)

This gives us in the \((t, x)\) plane the \( t_* \)-parametrized particle path, and by elimination of \( t_* \) we get it as \( x = x(t) \). We suggest to call this procedure "construction of a particle path by parametric subordination". Note that the process \( t = T(t_*) \) yielding the second random function in (6.3) has the properties of a subordinator in the sense of Definition 21.4 in [15].

Concerning notation: It is good to make a conceptual distinction between the position \( \bar{x} \) of an individual particle and the variable \( x \), likewise between
the physical time position \( \bar{t} \) and the physical time variable \( t \). When there are many particles we have overall densities for them and for these densities fractional diffusion equations. The pdf for the particle being in point \( \bar{x} = x \) at operational time \( t_* \), that we denote by \( \bar{u}_\beta(x, t_*) = f_{\alpha, \theta}(x, t_*) \), satisfies the evolution equation (Eq. (5.13) re-written with \( \bar{u}_\beta \))

\[
\frac{\partial}{\partial t_*} \bar{u}_\beta(x, t_*) = x D_\alpha^\beta \bar{u}_\beta(x, t_*), \quad \bar{u}(x, 0) = \delta(x).
\] (6.5)

The pdf for the physical time being in \( \bar{t} = t \) at operational time \( t_* \), that we denote by \( \bar{v}(t, t_*) = \bar{g}_\beta(t, t_*), \) obeys the skewed fractional equation

\[
\frac{\partial}{\partial t_*} \bar{v}(t, t_*) = t D_{-\beta} \bar{v}(t, t_*), \quad \bar{v}(t, 0) = \delta(t).
\] (6.6)

**Remark:** In operational time two Markovian random functions \( \bar{x}(t_*) \), \( \bar{t}(t_*) \) occur, as random processes, individually for each particle. In physical coordinates we have the \( t_* \)-parametrized random path described by (6.3).

**Remark:** It is instructive to see what happens for the limiting value \( \beta = 1 \). In this case the Laplace transform of \( \bar{g}_\beta(t, t_*) = \bar{g}_1(t, t_*) \) is \( \exp(-t s) \), implying \( \bar{g}_1(t, t_*) = \delta(t - t_*) \), the delta density concentrated on \( t = t_* \). So, in this case, \( t = t_* \), operational time and physical time coincide.

### 7 Numerical results

In this Section, after describing the numerical schemes adopted, we shall show the sample paths for four case studies of symmetric (\( \theta = 0 \)) fractional diffusion processes: \( \{\alpha = 2, \beta = 0.90\}, \{\alpha = 2, \beta = 0.80\}, \{\alpha = 1.5, \beta = 0.90\}, \{\alpha = 1.5, \beta = 0.80\} \). As explained in the previous Sections, for each case we need to construct the sample paths for three distinct processes, the parent process \( x = Y(t_*) \), the leading process \( t = T(t_*) \) (both in the operational time) and, finally, the subordinated process \( x = X(t) \), corresponding to the required fractional diffusion process. For this purpose we proceed as follows for the required three steps.

First, let the operational time \( t_* \) assume \( N \) discrete equidistant values in a given interval \([0, T]\), that is \( t_{*, n} = nT/N, \ n = 0, 1, \ldots, N \). As a working choice we take \( T = 1 \) and \( N = 10^6 \). Then produce \( N \) independent identically distributed (iid) random deviates, \( Y_1, Y_2, \ldots, Y_N \) having a symmetric stable probability distribution of order \( \alpha \), see the book by Janicki [23] for a useful and efficient method to do that. Now, with the points

\[
x_0 = 0, \quad x_n = \sum_{k=1}^{n} X_k, \quad n = 1, \ldots, N,
\] (7.1)
the couples \((t_n, x_n)\), plotted in the \((t, x)\) plane (operational time, physical space) can be considered as points of a true sample path \(\{x(t_s) : 0 \leq t_s \leq T\}\) of a symmetric Lévy motion with order \(\alpha\) corresponding to the integer values of operational time \(t_s = t_{s,n}\). In this identification of \(t_s\) with \(n\) we use the fact that our stable laws for waiting times and jumps imply \(\lambda = \mu = 1\) in the asymptotics \((5.1)\) and \((5.2)\) and \(\tau = h = 1\) as initial scaling factors in \((5.3)\) and \((5.14)\).

In order to complete the sample path we agree to connect every two successive points \((t_{s,n}, x_n)\) and \((t_{s,n+1}, x_{n+1})\) by a horizontal line from \((t_{s,n}, x_n)\) to \((t_{s,n+1}, x_n)\), and a vertical line from \((t_{s,n+1}, x_n)\) to \((t_{s,n+1}, x_{n+1})\). Obviously, this is not the 'true' Lévy motion from point \((t_{s,n}, x_n)\) to point \((t_{s,n+1}, x_{n+1})\), but from the theory of CTRW we know this kind of discrete random process to converge in the appropriate sense to Lévy motion. The points \((t_{s,n}, x_n)\) are points of a true Lévy motion.

As a second step, we produce \(N\) iid random deviates, \(T_1, T_2, \ldots, T_N\) having a stable probability distribution with order \(\beta\) and skewness \(-\beta\) (extremal stable distributions). Then, consider the points

\[ t_0 = 0, \quad t_n = \sum_{k=1}^{n} T_k, \quad n = 1, \ldots, N, \quad (7.2) \]

and plot the couples \((t_n, t_{s,n})\) in the \((t, t)\) (operational time, physical time) plane. By connecting points with horizontal and vertical lines we get sample paths \(\{t(t_s) : 0 \leq t_s \leq N\tau = 1\}\) describing the evolution of the physical time \(t\) with increasing operational time \(t_s\).

The final (third) step consists in plotting points \((t(t_{s,n}), x(t_{s,n}))\) in the \((t, x)\) plane, namely the physical time-space plane, and connecting them as before. So one gets a good approximation of the sample paths of the subordinated fractional diffusion process of parameters \(\alpha, \beta\) and \(\theta = 0\).

Now as the successive values of \(t_{s,n}\) and \(x_n\) are generated by successively adding the relevant standardized stable random deviates, the obtained sets of points in the three coordinate planes: \((t_s, t), (t_s, x), (t, x)\) can, in view of infinite divisibility and self-similarity of the stable probability distributions, be considered as snapshots of the corresponding true random processes occurring in continuous operational time \(t_s\) and physical time \(t\), correspondingly. Clearly, fine details between successive points are missing. They are hidden:

- In the \((t_s, x)\) plane in the horizontal lines from \((t_{s,n}, x_n)\) to \((t_{s,n+1}, x_n)\) and the vertical lines from \((t_{s,n+1}, x_n)\) to \((t_{s,n+1}, x_{n+1})\).
- In the \((t_s, t)\) plane in the horizontal lines from \((t_{s,n}, t_n)\) to \((t_{s,n+1}, t_n)\) and
the vertical lines from \((t_{s,n+1}, t_n)\) to \((t_{s,n+1}, t_{n+1})\).

- In the \((t, x)\) plane in the horizontal lines from \((t_n, x_n)\) to \((t_{n+1}, x_n)\) and the vertical lines from \((t_{n+1}, x_n)\) to \((t_{n+1}, x_{n+1})\).

The well-scaled passage to the diffusion limit here consists simply in regularly subdividing the \(\{t_s\}\) intervals of length 1 into smaller and smaller subintervals (all of equal length \(\tau\) and adjusting the random increments of \(t\) and \(x\) according to the requirement of self-similarity, namely taking, respectively, the waiting times and spatial jumps as \(\tau^{1/\beta}\) multiplied by a standard extreme \(\beta\)-stable deviate, \(\tau^{1/\alpha}\) multiplied by a standard (in our special case: symmetric) \(\alpha\)-stable deviate, respectively, as required by the self-similarity properties of the stable probability distributions). Furthermore if we watch sample path in a large interval of operational time \(t_s\), the points \((t_{s,n}, x_n)\) and \((t_{s,n+1}, x_{n+1})\) will in the graphs appear very near to each other in operational time \(t_s\) and aside from missing mutually cancelling jumps up and down (extremely near to each other) we have a good picture of the true processes.

The resulting sample paths for all the processes involved in the two case studies are presented in the Figs. 1-6. The figure captions should clarify our strategy. Figs. 1 and 4 are referring to the parent processes characterized by the parameter \(\alpha = 2\) and \(\alpha = 1.5\). Figs. 2 and 5 are devoted to the leading processes \(t^*_s\) characterized by the parameter \(\beta = 0.9\) and \(\beta = 0.8\) in the Right and Left plates, respectively. As a consequence Figures 2 and 5 are identical, because are referring to the same processes. Finally, Figs. 3 and 6 are devoted to the subordinated processes resulting from the previous parent and leading processes. Specifically in Fig. 3 the Left and Right plates show sample paths for \(\alpha = 2\) and \(\beta = 0.9, 0.8\), respectively, and in Fig. 6 the Left and Right plates show sample paths for \(\alpha = 1.5\) and \(\beta = 0.9, 0.8\), respectively.

By observing the figures the reader will note that horizontal segments (waiting times) in the \((t, x)\) plane (Fig. 3, Fig. 6) correspond to vertical segments (jumps) in the \((t, t^*_s)\) plane (Fig. 2, Fig. 5). Actually, the graphs in the \((t, x)\)-plane depict continuous time random walks with waiting times \(T_k\) (shown as horizontal segments) and jumps \(X_k\) (shown as vertical segments). The left endpoints of the horizontal segments can be considered as snapshots of the true particle path (the true random process to be simulated), the

\footnote{Figs. 2 and 5 alternatively can also be viewed as graphical representations of the directing processes \(t^*_s = T^*_s(t)\) in the sense of Feller, see Section 4. We note that the directing processes, exhibiting horizontal segments, are no longer Lévy processes even if the random functions \(t^*_s = T^*_s(t)\) are non-decreasing and right-continuous like the leading processes \(t = T(T^*_s)\). This explains the non-Markovianity of the subordinated processes.}
Figure 1: A sample path for the parent process \( x = Y(t_*) \) with \( \{\alpha = 2\} \).

Figure 2: A sample path for the leading process \( t = T(t_*) \).
LEFT: \( \{\beta = 0.90\} \), RIGHT: \( \{\beta = 0.80\} \).

Figure 3: A sample path for the subordinated process \( x = X(t) \).
LEFT: \( \{\alpha = 2, \beta = 0.90\} \), RIGHT: \( \{\alpha = 2, \beta = 0.80\} \).
Figure 4: A sample path for the parent process $x = Y(t_*)$ with $\{\alpha = 1.5\}$.

Figure 5: A sample path for the leading process $t = T(t_*)$.
LEFT: $\{\beta = 0.90\}$, RIGHT: $\{\beta = 0.80\}$.

Figure 6: A sample path for the subordinated process $x = X(t)$.
LEFT: $\{\alpha = 1.5, \beta = 0.90\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.80\}$.
segments being segments of our ignorance. In the interval $t_n < t \leq t_{n+1}$ the true process (namely the spatial variable $x = X(t)$) may jump up and down (infinitely) often, the sum (or integral) of all these ups (counted positive) and downs (counted negative) amounting to the vertical jump $X_{n+1}$.

Finer details will become visible by choosing in the operational time $t_*$ the step length $\tau$ smaller and smaller. In the graphs we can clearly see what happens for finer and finer discretization of the operational time $t_*$, by adopting $10^1$, $10^2$, $10^3$ steps, see Figures 7-18. As a matter of fact there is no visible difference in the transition for the successive decades $10^4$, $10^5$, $10^6$ steps as the great majority of spatial jumps and waiting times are very small. This property also explains the visible persistence of large jumps and waiting times even of very small steps $\tau$ of the operational time.

8 Conclusions

Starting from the series representation (3.5) of the CTRW, by considering there the running index of summation as discrete operational time and passing to the diffusion limit in a well-scaled way, we have shown how to arrive at the integral formula of subordination in fractional diffusion. Furthermore, we have explained how, in analogy to the construction of particle paths in CTRW, particle paths in space-time fractional diffusion can be obtained by composition of two stable (hence Markovian) processes (one for the physical time, the other for the position in space, both processes running in operational time). By this composition we get in physical space-time the particle path, parametrized by the operational time. For this construction of a particle path we suggest the name parametric subordination. The essential games are played in operational time, for construction of a particle path we avoid to explicitly run the hitting time process (see [32]) generating from physical time the operational time.

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Figure 7: A sample path for the parent process $x = Y(t_\ast)$. 
LEFT: $\{\alpha = 2, N = 10^1\}$, RIGHT: $\{\alpha = 1.5, N = 10^1\}$.

Figure 8: A sample path for the parent process $x = Y(t_\ast)$. 
LEFT: $\{\alpha = 2, N = 10^2\}$, RIGHT: $\{\alpha = 1.5, N = 10^2\}$.

Figure 9: A sample path for the parent process $x = Y(t_\ast)$. 
LEFT: $\{\alpha = 2, N = 10^3\}$, RIGHT: $\{\alpha = 1.5, N = 10^3\}$. 
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Figure 10: A sample path for the leading process $t = T(t_*)$.
LEFT: $\{\beta = 0.9, \ N = 10^1\}$, RIGHT: $\{\beta = 0.8, \ N = 10^1\}$.

Figure 11: A sample path for the leading process $t = T(t_*)$.
LEFT: $\{\beta = 0.9, \ N = 10^2\}$, RIGHT: $\{\beta = 0.8, \ N = 10^2\}$.

Figure 12: A sample path for the leading process $t = T(t_*)$.
LEFT: $\{\beta = 0.9, \ N = 10^3\}$, RIGHT: $\{\beta = 0.8, \ N = 10^3\}$.
Figure 13: A sample path for the subordinated process \( x = X(t) \).
LEFT: \( \{ \alpha = 2, \beta = 0.90, N = 10^1 \} \), RIGHT: \( \{ \alpha = 2, \beta = 0.80, N = 10^1 \} \).

Figure 14: A sample path for the subordinated process \( x = X(t) \).
LEFT: \( \{ \alpha = 2, \beta = 0.90, N = 10^2 \} \), RIGHT: \( \{ \alpha = 2, \beta = 0.80, N = 10^2 \} \).

Figure 15: A sample path for the subordinated process \( x = X(t) \).
LEFT: \( \{ \alpha = 2, \beta = 0.90, N = 10^3 \} \), RIGHT: \( \{ \alpha = 2, \beta = 0.80, N = 10^3 \} \).
Figure 16: A sample path for the subordinated process $x = X(t)$.
LEFT: $\{\alpha = 1.5, \beta = 0.90, N = 10^1\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.80, N = 10^1\}$.

Figure 17: A sample path for the subordinated process $x = X(t)$.
LEFT: $\{\alpha = 1.5, \beta = 0.90, N = 10^2\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.80, N = 10^2\}$.

Figure 18: A sample path for the subordinated process $x = X(t)$.
LEFT: $\{\alpha = 1.5, \beta = 0.90, N = 10^3\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.80, N = 10^3\}$.
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