Parametric subordination in fractional diffusion processes

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Abstract
We consider simulation of spatially one-dimensional space-time fractional diffusion. Whereas in an earlier paper of ours (Eur. Phys. J. Special Topics, Vol. 193, 119–132 (2011); E-print: \text{http://arxiv.org/abs/1104.4041}), we have developed the basic theory of what we call parametric subordination via three-fold splitting applied to continuous time random walk with subsequent passage to the diffusion limit, here we go the opposite way. Via Fourier-Laplace manipulations of the relevant fractional partial differential equation of evolution we obtain the subordination integral formula that teaches us how a particle path can be constructed by first generating the operational time from the physical time and then generating in operational time the spatial path. By inverting the generation of operational time from physical time we arrive at the method of parametric subordination. Due to the infinite divisibility of the stable subordinator we can simulate particle paths by discretization where the generated points of a path are precise snapshots of a true path. By refining the discretization more and more fine details of a path become visible.

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## Contents

1 Introduction .................................................. 3

2 Notions and Notations ........................................... 4
   2.1 The Fourier transform ..................................... 4
   2.2 The Laplace transform .................................... 5
   2.3 The auxiliary functions of Mittag-Leffler type ....... 5
   2.4 The auxiliary functions of the Wright type .......... 7
   2.5 The Lévy stable distributions ............................. 10

3 The Space-Time Fractional Diffusion ......................... 15
   3.1 The Riesz-Feller space-fractional derivative .......... 15
   3.2 The Caputo fractional derivative ........................ 16
   3.3 The fundamental solution of the space-time fractional diffusion equation ................................. 17
   3.4 Alternative forms of the space-time fractional diffusion equation ................................................. 18

4 Analytic and stochastic pathways to subordination in space-time fractional diffusion ......................... 20
   4.1 The analytical interpretation via operational time. . . 20
   4.2 Stochastic interpretation .................................. 22
   4.3 Evolution equations for the densities \( r_\beta(t, t_*) \) of \( t = t(t_*) \) and \( q_\beta(t_*, t) \) of \( t_* = t_*(t) \) .................................................. 24
   4.4 The random walks ......................................... 25

5 Graphical representations and Conclusions ................... 27
   Acknowledgements ............................................ 34
   References .................................................... 34
1 Introduction

The purpose of this chapter is to describe our method of parametric subordination to produce particle trajectories for the so-called fractional diffusion processes.

By replacing in the common diffusion equation the first order time derivative and the second order space derivative by appropriate fractional derivatives we obtain a fractional diffusion equation whose solution describes the temporal evolution of the density of an extensive quantity, e.g. of the sojourn probability of a diffusing particle.

After giving a survey on analytic methods for determination of the solution (this is the macroscopic aspect) we turn attention to the problem of simulation of particle trajectories (the microscopic aspect). By some authors such simulation is called ”particle tracking”, see e.g. [65].

As an approximate method among physicists the so-called Continuous Time Random Walk (CTRW) is very popular. On the other hand, it is possible to produce a sequence of precise snapshots of a true trajectory. This is achieved by a change from the ”physical time” to an ”operational time” in which the simulation is carried out. By two Markov processes happening in operational time the running of physical time and the motion in space are produced. Then, elimination of the operational time yields a picture of the desired trajectory. It is remarkable that so by combination of two Markov processes a non-Markovian process is generated.

The two Markov processes can be obtained and analyzed in two ways:
(a) from the CTRW model by a well-scaled passage to the ”diffusion limit”,
(b) directly from an integral representation of the fundamental solution of the fractional diffusion equation.

We have developed way (a) in our 2007 paper [18] via passage to the diffusion limit in the Cox-Weiss solution formula for CTRW and by the technique of splitting the CTRW into three separate walks and passing in each of these to the diffusion limit in our more recent paper [17]. For another access (more oriented towards measure-theoretic theory of stochastic processes) see the recent papers [19, 20]. In [20] the authors also treat the problem of subordination for diffusion with distributed orders of time-fractional differentiation.
The plan of our chapter is as follows. In Section 2 we provide for the reader’s convenience some preliminary notions and notations as a mathematical background for our further analysis. In Section 3 we introduce the space-time fractional diffusion equation, based on the Riesz-Feller and Caputo fractional derivatives, and we present the fundamental solution.. In Section 4 we provide the stochastic interpretation of the space-time fractional diffusion equation discussing the concepts of subordination, the main goal of this chapter. Finally, in Section 5 we show some graphical representations along with conclusions.

2 Notions and Notations

In this Section we survey some preliminary notions including Fourier and Laplace transforms, special functions of Mittag-Leffler and Wright type and Lévy stable probability distributions.

Since in what follows we shall meet only real or complex-valued functions of a real variable that are defined and continuous in a given open interval $I = (a, b)$, $-\infty \leq a < b \leq +\infty$, except, possibly, at isolated points where these functions can be infinite, we restrict our presentation of the integral transforms to the class of functions for which the Riemann improper integral on $I$ absolutely converges. In so doing we follow Marichev [33] and we denote this class by $L^c(I)$ or $L^c(a, b)$.

2.1 The Fourier transform

Let

$$\hat{f}(\kappa) = \mathcal{F} \{ f(x); \kappa \} = \int_{-\infty}^{+\infty} e^{+ix\kappa} f(x) \, dx, \quad \kappa \in \mathbb{R},$$

(2.1a)

be the Fourier transform of a function $f(x) \in L^c(I)$, and let

$$f(x) = \mathcal{F}^{-1} \{ \hat{f}(\kappa); x \} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{-ix\kappa} \hat{f}(\kappa) \, d\kappa, \quad x \in \mathbb{R},$$

(2.1b)

be the inverse Fourier transform.

If $f(x)$ is piecewise differentiable, then the formula (2.1b) holds true at all points where $f(x)$ is continuous and the integral in it must be understood in the sense of the Cauchy principal value.
Related to the Fourier transform is the notion of pseudo-differential operator. Let us recall that a generic pseudo-differential operator $A$, acting with respect to the variable $x \in \mathbb{R}$, is defined through its Fourier representation, namely

$$
\int_{-\infty}^{+\infty} e^{ix\xi} A[f(x)] \, dx = \hat{A}(\xi) \hat{f}(\xi), \quad (2.2)
$$

where $\hat{A}(\xi)$ is referred to as symbol of $A$, formally given as

$$
\hat{A}(\xi) = (A e^{-i\xi x}) e^{+i\xi x}.
$$

### 2.2 The Laplace transform

Let

$$
\tilde{f}(s) = \mathcal{L}\{f(t); s\} = \int_0^{+\infty} e^{-st} f(t) \, dt, \quad \text{Re}(s) > a_f, \quad (2.3a)
$$

be the Laplace transform of a function $f(t) \in \mathcal{L}^c(0, T), \forall T > 0$ and let

$$
f(t) = \mathcal{L}^{-1}\{\tilde{f}(s); t\} = \frac{1}{2\pi i} \int_{\gamma-i\infty}^{\gamma+i\infty} e^{st} \tilde{f}(s) \, ds, \quad \text{Re}(s) = \gamma > a_f, \quad (2.3b)
$$

with $t > 0$, be the inverse Laplace transform.

### 2.3 The auxiliary functions of Mittag-Leffler type

The Mittag-Leffler functions, that we denote by $E_{\alpha}(z), E_{\alpha,\beta}(z)$ are so named in honour of Gösta Mittag-Leffler, the eminent Swedish mathematician, who introduced and investigated these functions in a series of notes starting from 1903 in the framework of the theory of entire functions. The functions are defined by the series representations, convergent in the whole complex plane $\mathbb{C}$

$$
E_{\alpha}(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + 1)}, \quad \text{Re}(\alpha) > 0; \quad (2.4)
$$

A sufficient condition of the existence of the Laplace transform is that the original function is of exponential order as $t \to \infty$. This means that some constant $a_f$ exists such that the product $e^{-a_f t} |f(t)|$ is bounded for all $t$ greater than some $T$. Then $\tilde{f}(s)$ exists and is analytic in the half plane $\text{Re}(s) > a_f$. If $f(t)$ is piecewise differentiable, then the formula (2.3b) holds true at all points where $f(t)$ is continuous and the (complex) integral in it must be understood in the sense of the Cauchy principal value.
\[ E_{\alpha,\beta}(z) := \sum_{n=0}^{\infty} \frac{z^n}{\Gamma(\alpha n + \beta)}, \quad \text{Re}(\alpha) > 0, \ \beta \in \mathbb{C}. \] (2.5)

Originally Mittag-Leffler assumed only the parameter \( \alpha \) and assumed it as positive, but soon later the generalization with two complex parameters was considered by Wiman. In both cases the Mittag-Leffler functions are entire of order \( 1/\text{Re}(\alpha) \). Generally \( E_{\alpha,1}(z) = E_{\alpha}(z) \).

Using their series representations it is easy to recognize

\[
\begin{align*}
E_{1,1}(z) &= E_1(z) = e^z, & E_{1,2}(z) &= \frac{e^z - 1}{z}, \\
E_{2,1}(z^2) &= \cosh(z), & E_{2,1}(-z^2) &= \cos(z), \\
E_{2,2}(z^2) &= \frac{\sinh(z)}{z}, & E_{2,2}(-z^2) &= \frac{\sin(z)}{z},
\end{align*}
\] (2.6)

and more generally

\[
\begin{align*}
E_{\alpha,\beta}(z) + E_{\alpha,\beta}(-z) &= 2 E_{2\alpha,\beta}(z^2), \\
E_{\alpha,\beta}(z) - E_{\alpha,\beta}(-z) &= 2z E_{2\alpha,\alpha+\beta}(z^2).
\end{align*}
\] (2.7)

We note that in Chapter 18 of Vol. 3 of the handbook of the 1955 Bateman Project devoted to Miscellaneous Functions, we find a valuable survey of these functions, which later were recognized as belonging to the more general class of Fox \( H \)-functions introduced after 1960.

For our purposes relevant roles are played by the following auxiliary functions of the Mittag-Leffler type on support \( \mathbb{R}^+ \) defined as follows, where \( \lambda > 0 \), along with their Laplace transforms

\[
e_{\alpha}(t; \lambda) := E_{\alpha}(-\lambda t^\alpha) \div \frac{s^{\alpha-1}}{s^\alpha + \lambda}, \] (2.8)

\[
e_{\alpha,\beta}(t; \lambda) := t^{\beta-1} E_{\alpha,\beta}(-\lambda t^\alpha) \div \frac{s^{\alpha-\beta}}{s^\alpha + \lambda}, \] (2.9)

\[
e_{\alpha,\alpha}(t; \lambda) := t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^\alpha) = \frac{d}{dt} e_{\alpha}(-\lambda t^\alpha) = \div - \frac{\lambda}{s^\alpha + \lambda}, \] (2.10)

Here we have used the sign \( \div \) for the juxtaposition of a function depending on \( t \) with its Laplace transform depending on \( s \). Later we use this sign also for juxtaposition of a function depending on \( x \) with its Fourier transform depending on \( \kappa \).
Remark: We outline that the above auxiliary functions (for restricted values of the parameters) turn out to be completely monotone (CM) functions so that they enter in some types of relaxation phenomena of physical relevance. We recall that a function \( f(t) \) is CM in \( \mathbb{R}^+ \) if \((-1)^n f^n(t) \geq 0\). The function \( e^{-t} \) is the prototype of a CM function. For a Bernstein theorem, more generally they are expressed in terms of a (generalized) real Laplace transform of a positive measure

\[
 f(t) = \int_0^\infty e^{-rt} K(r) \, dr, \quad K(r) \geq 0. \tag{2.11}
\]

Restricting attention to the auxiliary function in two parameters, we can prove for \( \lambda > 0 \) that

\[
e_{\alpha,\beta}(t; \lambda) := t^{\beta - 1} E_{\alpha,\beta}(-\lambda t^\alpha) \quad \text{CM} \iff 0 < \alpha \leq \beta \leq 1. \tag{2.12}
\]

Using the Laplace transform we can prove, following Gorenflo and Mainardi \[13\], that for \( 0 < \alpha < 1 \) and \( \lambda = 1 \)

\[
 E_\alpha(-t^\alpha) \simeq \begin{cases} 
 1 - \frac{t^\alpha}{\Gamma(\alpha + 1)} + \frac{t^{2\alpha}}{\Gamma(2\alpha + 1)} & t \to 0^+,
 
 \frac{t^{-\alpha}}{\Gamma(1 - \alpha)} - \frac{t^{-2\alpha}}{\Gamma(1 - 2\alpha)} & t \to +\infty,
\end{cases} \tag{2.13}
\]

and

\[
 E_\alpha(-t^\alpha) = \int_0^\infty e^{-rt} K_\alpha(r) \, dr \tag{2.14}
\]

with

\[
 K_\alpha(r) = \frac{1}{\pi} \frac{r^{-\alpha - 1} \sin(\alpha \pi)}{r^{2\alpha} + 2r^\alpha \cos(\alpha \pi) + 1} = \frac{1}{\pi} \frac{\sin(\alpha \pi)}{r^\alpha + 2 \cos(\alpha \pi) + r^{-\alpha}} > 0. \tag{2.15}
\]

2.4 The auxiliary functions of the Wright type

The Wright function, that we denote by \( W_{\lambda,\mu}(z) \), is so named in honour of E. Maitland Wright, the eminent British mathematician, who introduced and investigated this function in a series of notes starting from 1933 in the framework of the asymptotic theory of partitions, see \[61\] \[62\] \[63\]. The function is defined by the series representation, convergent in the whole \( z \)-complex plane \( \mathbb{C} \),

\[
 W_{\lambda,\mu}(z) := \sum_{n=0}^{\infty} \frac{z^n}{n! \Gamma(\lambda n + \mu)}, \quad \lambda > -1, \ \mu \in \mathbb{C}. \tag{2.16}
\]
Originally, Wright assumed $\lambda \geq 0$, and, only in 1940 [64], he considered $-1 < \lambda < 0$. We note that in Chapter 18 of Vol. 3 of the handbook of the 1955 Bateman Project [5] devoted to Miscellaneous Functions, we find an earlier analysis of these functions, which, similarly with the Mittag-Leffler functions, were later recognized as belonging to the more general class of Fox $H$-functions introduced after 1960. However, in that Chapter, presumably for a misprint, the parameter $\lambda$ of the Wright function is restricted to be nonnegative. It is possible to prove that the Wright function is entire of order $1/(1 + \lambda)$, hence it is of exponential type only if $\lambda \geq 0$. For this reason we propose to distinguish the Wright functions in two kinds according to $\lambda \geq 0$ (first kind) and $-1 < \lambda < 0$ (second kind). Both kinds of functions are related to the Mittag-Leffler function via Laplace transform pairs: in fact we have, see for details the appendix F of the recent book by Mainardi [28], for the case $\lambda > 0$ (Wright functions of the first kind)

$$W_{\lambda, \mu}(\pm r) \div \frac{1}{s} E_{\lambda, \mu} \left( \pm \frac{1}{s} \right), \quad \lambda > 0,$$  

(2.17)

and for the case $\lambda = -\nu \in (-1, 0)$ (Wright functions of the second kind),

$$W_{-\nu, \mu}(-r) \div E_{\nu, \mu + \nu}(-s), \quad 0 < \nu < 1.$$  

(2.18)

For our purposes relevant roles are played by the following auxiliary functions of the Wright type (of the second kind)

$$F_{\nu}(z) := W_{-\nu, 0}(-z) = \sum_{n=1}^{\infty} \frac{(-z)^n}{n! \Gamma(-\nu n)}, \quad 0 < \nu < 1,$$  

(2.19)

and

$$M_{\nu}(z) := W_{-\nu, 1-\nu}(-z) = \sum_{n=0}^{\infty} \frac{(-z)^n}{n! \Gamma[-\nu n + (1 - \nu)]}, \quad 0 < \nu < 1,$$  

(2.20)

interrelated through $F_{\nu}(z) = \nu z M_{\nu}(z)$. The relevance of these functions was pointed out by Mainardi in his former analysis of the time fractional diffusion equation via Laplace transform. Restricting our attention to the $M$-Wright functions on support $\mathbb{R}^+$ we point out the Laplace transforms pairs

$$M_{\nu}(r) \div E_{\nu}(-s), \quad 0 < \nu < 1.$$  

(2.21)
\[
\frac{\nu}{r^{\nu+1}} M_\nu(1/r^\nu) \div e^{-s^\nu}, \quad 0 < \nu < 1.
\] (2.22)

\[
\frac{1}{r^\nu} M_\nu(1/r^\nu) \div \frac{e^{-s^\nu}}{s^{1-\nu}}, \quad 0 < \nu < 1.
\] (2.23)

It was also proved in [28] that the \( M \)-Wright function on support \( \mathbb{R}^+ \) is a probability density function (pdf) that in the literature is sometimes known as the density related to Mittag-Leffler probability distribution. Its absolute moments of order \( \delta > -1 \) in \( \mathbb{R}^+ \) are finite and turn out to be

\[
\int_0^\infty r^\delta M_\nu(r) \, dr = \frac{\Gamma(\delta + 1)}{\Gamma(\nu \delta + 1)}, \quad \delta > -1, \quad 0 \leq \nu < 1.
\] (2.24)

We point out that in the limit \( \nu \to 1^- \) the function \( M_\nu(r) \), for \( r \in \mathbb{R}^+ \), tends to the Dirac generalized function \( \delta(r - 1) \).

For our next purposes it is worthwhile to introduce the function in two variables

\[
M_\nu(x,t) := t^{-\nu} M_\nu(x t^{-\nu}), \quad 0 < \nu < 1, \quad x, t \in \mathbb{R}^+,
\] (2.25)

which defines a spatial probability density in \( x \) evolving in time \( t \) with self-similarity exponent \( H = \nu \). Of course for \( x \in \mathbb{R} \) we can consider the symmetric version obtained from (2.25) multiplying by 1/2 and replacing \( x \) by \( |x| \). Hereafter we provide a list of the main properties of this density, which can be derived from the Laplace and Fourier transforms for the corresponding Wright \( M \)-function in one variable.

From Eq. (2.23) we derive the Laplace transform of \( M_\nu(x,t) \) with respect to \( t \in \mathbb{R}^+ \),

\[
\mathcal{L} \{ M_\nu(x,t); t \to s \} = s^{\nu-1} e^{-xs^\nu}.
\] (2.26)

From Eq. (2.21) we derive the Laplace transform of \( M_\nu(x,t) \) with respect to \( x \in \mathbb{R}^+ \),

\[
\mathcal{L} \{ M_\nu(x,t); x \to s \} = E_\nu(-st^\nu) .
\] (2.27)

From the recent book by Mainardi [28] we recall the Fourier transform of \( M_\nu(|x|, t) \) with respect to \( x \in \mathbb{R} \),

\[
\mathcal{F} \{ M_\nu(|x|, t); x \to \kappa \} = 2 E_{2\nu} \left( -\kappa^2 t^{2\nu} \right),
\] (2.28)
and, in particular,

\[
\begin{align*}
\int_0^\infty \cos(\kappa x) M_\nu(x, t) \, dx &= E_{2\nu,1}(-\kappa^2 t^{2\nu}), \\
\int_0^\infty \sin(\kappa x) M_\nu(x, t) \, dx &= \kappa t^\nu E_{2\nu,1+\nu}(-\kappa^2 t^{2\nu}).
\end{align*}
\] (2.29)

It is worthwhile to note that for \( \nu = 1/2 \) we recover the Gaussian density evolving with time with variance \( \sigma^2 = 2t \)

\[
\frac{1}{2} M_{1/2}(x, t) = \frac{1}{2\sqrt{\pi} t^{1/2}} e^{-x^2/(4t)}.
\] (2.30)

2.5 The Lévy stable distributions

The term stable has been assigned by the French mathematician Paul Lévy, who, in the twenties of the last century, started a systematic research in order to generalize the celebrated Central Limit Theorem to probability distributions with infinite variance. For stable distributions we can assume the following DEFINITION: If two independent real random variables with the same shape or type of distribution are combined linearly with positive coefficients and the distribution of the resulting random variable has the same shape, the common distribution (or its type, more precisely) is said to be stable.

The restrictive condition of stability enabled Lévy (and then other authors) to derive the canonic form for the characteristic function of the densities of these distributions. Here we follow the parameterization by Feller\[6 \] revisited in \[14\] and in \[29\]. Denoting by \( L_\alpha^\theta(x) \) a generic stable density in \( \mathbb{R} \), where \( \alpha \) is the index of stability and and \( \theta \) the asymmetry parameter, improperly called skewness, its characteristic function reads:

\[
\begin{align*}
L_\alpha^\theta(x) \div \tilde{L}_\alpha^\theta(\kappa) &= \exp \left[-\psi_\alpha^\theta(\kappa)\right], \quad \psi_\alpha^\theta(\kappa) = |\kappa|^\alpha e^{i \text{sign}(\kappa) \theta \pi/2}, \\
0 < \alpha \leq 2, \quad |\theta| &\leq \min \left\{ \alpha, 2 - \alpha \right\}.
\end{align*}
\] (2.31)

We note that the allowed region for the real parameters \( \alpha \) and \( \theta \) turns out to be a diamond in the plane \( \{\alpha, \theta\} \) with vertices in the points \((0,0), (1,1), (1,-1), (2,0)\), that we call the Feller-Takayasu diamond, see Figure [14]. For values of \( \theta \) on the border of the diamond (that is \( \theta = \pm \alpha \) if \( 0 < \alpha < 1 \), and \( \theta = \pm (2 - \alpha) \) if \( 1 < \alpha < 2 \)) we obtain the so-called extremal stable densities.
We note the symmetry relation \( L_{\theta}^{-\theta}(-x) = L_{\theta}(x) \), so that a stable density with \( \theta = 0 \) is symmetric.

Stable distributions have noteworthy properties on which the interested reader can be informed from the relevant existing literature. Hereafter we recall some peculiar properties:

- Each stable density \( L_{\alpha}^{\theta} \) possesses a domain of attraction, see e.g. [6].
- Any stable density is unimodal and indeed bell-shaped, i.e. its \( n \)-th derivative has exactly \( n \) zeros in \( \mathbb{R} \), see [10].
- The stable distributions are self-similar and infinitely divisible.

These properties derive from the canonic form (2.31) through the scaling property of the Fourier transform.

**Self-similarity** means

\[
L_{\alpha}^{\theta}(x,t) \stackrel{\mathcal{F}}{=} \exp \left[ -t\psi_{\alpha}(\kappa) \right] \iff L_{\alpha}^{\theta}(x,t) = t^{-1/\alpha} L_{\alpha}^{\theta}(x/t^{1/\alpha}) \, , \tag{2.32}
\]

where \( t \) is a positive parameter. If \( t \) is time, then \( L_{\alpha}^{\theta}(x,t) \) is a spatial density evolving in time with self-similarity.

**Infinite divisibility** means that for every positive integer \( n \), the characteristic function can be expressed as the \( n \)-th power of some characteristic function, so that any stable distribution can be expressed as the \( n \)-fold convolution of a stable distribution of the same type. Indeed, taking in (2.31) \( \theta = 0 \),
without loss of generality, we have
\[ e^{-t|\kappa|^\alpha} = [e^{-(t/n)|\kappa|^\alpha}]^n \iff L_\alpha^0(x, t) = [L_\alpha^0(x, t/n)]^{*n} \], \tag{2.33}

where
\[ [L_\alpha^0(x, t/n)]^{*n} := L_\alpha^0(x, t/n) \ast L_\alpha^0(x, t/n) \ast \cdots \ast L_\alpha^0(x, t/n) \tag{2.34} \]
is the multiple Fourier convolution in \( \mathbb{R} \) with \( n \) identical terms.

Only in special cases the inversion of the Fourier transform in (2.31) can be carried out using standard tables, and provides well-known probability distributions.

For \( \alpha = 2 \) (so \( \theta = 0 \)), we recover the Gaussian pdf, that turns out to be the only stable density with finite variance, and more generally with finite moments of any order \( \delta \geq 0 \). In fact
\[ L_2^0(x) = \frac{1}{2\sqrt{\pi}}e^{-x^2/4}. \tag{2.35} \]

All the other stable densities have finite absolute moments of order \( \delta \in [-1, \alpha) \) as we will later show.

For \( \alpha = 1 \) and \( |\theta| < 1 \), we get
\[ L_1^\theta(x) = \frac{1}{\pi} \frac{\cos(\theta \pi/2)}{[x + \sin(\theta \pi/2)]^2 + [\cos(\theta \pi/2)]^2}, \tag{2.36} \]
which for \( \theta = 0 \) includes the Cauchy-Lorentz pdf,
\[ L_1^0(x) = \frac{1}{\pi} \frac{1}{1 + x^2}. \tag{2.37} \]

In the limiting cases \( \theta = \pm 1 \) for \( \alpha = 1 \) we obtain the singular Dirac pdf’s
\[ L_1^{\pm 1}(x) = \delta(x \pm 1). \tag{2.38} \]

In general, we must recall the power series expansions provided in \[6\]. We restrict our attention to \( x > 0 \) since the evaluations for \( x < 0 \) can be obtained using the symmetry relation. The convergent expansions of \( L_\alpha^0(x) \) (\( x > 0 \)) turn out to be;
for $0 < \alpha < 1$, $|\theta| \leq \alpha$:

$$L^\theta_\alpha(x) = \frac{1}{\pi x} \sum_{n=1}^{\infty} (-x^{-\alpha})^n \frac{\Gamma(1+n\alpha)}{n!} \sin \left[ \frac{n\pi}{2} (\theta - \alpha) \right] ; \quad (2.39)$$

for $1 < \alpha \leq 2$, $|\theta| \leq 2 - \alpha$:

$$L^\theta_\alpha(x) = \frac{1}{\pi x} \sum_{n=1}^{\infty} (-x)^n \frac{\Gamma(1+n/\alpha)}{n!} \sin \left[ \frac{n\pi}{2\alpha} (\theta - \alpha) \right] . \quad (2.40)$$

From the series in (2.39) and the symmetry relation we note that the extremal stable densities for $0 < \alpha < 1$ are unilateral, precisely vanishing for $x > 0$ if $\theta = \alpha$, vanishing for $x < 0$ if $\theta = -\alpha$. In particular the unilateral extremal densities $L^-_\alpha(x)$ with $0 < \alpha < 1$ have support $\mathbb{R}^+$ and Laplace transform $\exp(-s\alpha)$. For $\alpha = 1/2$ we obtain the so-called Lévy-Smirnov pdf:

$$L^{-1/2}_{1/2}(x) = \frac{x^{-3/2}}{2\sqrt{\pi}} e^{-1/(4x)} , \quad x \geq 0 . \quad (2.41)$$

It is worth to note that the Gaussian pdf (2.35) and the Lévy-Smirnov pdf (2.41) are well known in the treatment of the Brownian motion: the former as the spatial density on an infinite real line, the latter as the first passage time density on a semi-infinite line, see e.g. [6].

As a consequence of the convergence of the series in (2.39)-(2.40) and of the symmetry relation we recognize that the stable pdf’s with $1 < \alpha \leq 2$ are entire functions, whereas with $0 < \alpha < 1$ have the form

$$L^\theta_\alpha(x) = \begin{cases} (1/x) \Phi_1(x^{-\alpha}) & \text{for } x > 0 , \\ (1/|x|) \Phi_2(|x|^{-\alpha}) & \text{for } x < 0 , \end{cases} \quad (2.42)$$

where $\Phi_1(z)$ and $\Phi_2(z)$ are distinct entire functions. The case $\alpha = 1$ with $|\theta| < 1$ must be considered in the limit for $\alpha \to 1$ of (2.39)-(2.40), because the corresponding series reduce to power series akin with geometric series in $1/x$ and $x$, respectively, with a finite radius of convergence. The corresponding stable densities are no longer represented by entire functions, as can be noted directly from their explicit expressions (2.36)-(2.37).

From a comparison between the series expansions in (2.39)-(2.40) and in (2.19)-(2.20), we recognize that for $x > 0$ our auxiliary functions of the
Wright type are related to the extremal stable densities as follows, see [32],

\[ L^{-\alpha}_\alpha(x) = \frac{1}{x} F_\alpha(x^{-\alpha}) = \frac{\alpha}{x^{\alpha+1}} M_\alpha(x^{-\alpha}), \quad 0 < \alpha < 1, \]  
(2.43)

\[ L^{-2\alpha}_\alpha(x) = \frac{1}{x} F_{1/\alpha}(x) = \frac{1}{\alpha} M_{1/\alpha}(x), \quad 1 < \alpha \leq 2. \]  
(2.44)

In the above equations, for \( \alpha = 1 \), the skewness parameter turns out to be \( \theta = -1 \), so we get the singular limit

\[ L^{-1}_1(x) = M_1(x) = \delta(x - 1). \]  
(2.45)

We do not provide here the asymptotic representations of the stable densities referring the interested reader to [29]. However, based on asymptotic representations, we can state the following: For \( 0 < \alpha < 2 \) the stable densities exhibit \textit{fat tails} in such a way that their absolute moment of order \( \delta \) is finite only if \( -1 < \delta < \alpha \). More precisely, one can show that for non-Gaussian, not extremal, stable densities the asymptotic decay of the tails is

\[ L^\theta_\alpha(x) = O\left( |x|^{-(\alpha+1)} \right), \quad x \to \pm \infty. \]  
(2.46)

For the extremal densities with \( \alpha \neq 1 \) this is valid only for one tail (as \( |x| \to \infty \)), the other (as \( |x| \to \infty \)) being of exponential order. For \( 1 < \alpha < 2 \) the extremal pdf’s are two-sided and exhibit an exponential left tail (as \( x \to -\infty \)) if \( \theta = +(2 - \alpha) \), or an exponential right tail (as \( x \to +\infty \)) if \( \theta = -(2 - \alpha) \). Consequently, the Gaussian pdf is the unique stable density with finite variance. Furthermore, when \( 0 < \alpha \leq 1 \), the first absolute moment is infinite so we should use the median instead of the non-existent expected value in order to characterize the corresponding pdf.

Let us also recall a relevant identity between stable densities with index \( \alpha \) and \( 1/\alpha \) (a sort of reciprocity relation) pointed out in [6], that is, assuming \( x > 0 \),

\[ \frac{1}{x^{\alpha+1}} L^\theta_{1/\alpha}(x^{-\alpha}) = L^\theta_\alpha(x), \quad 1/2 \leq \alpha \leq 1, \quad \theta^* = \alpha(\theta + 1) - 1. \]  
(2.47)

The condition \( 1/2 \leq \alpha \leq 1 \) implies \( 1 \leq 1/\alpha \leq 2 \). A check shows that \( \theta^* \) falls within the prescribed range \( |\theta^*| \leq \alpha \) if \( |\theta| \leq 2 - 1/\alpha \). We leave as an exercise for the interested reader the verification of this reciprocity relation in the limiting cases \( \alpha = 1/2 \) and \( \alpha = 1 \). For more details on Lévy stable densities
we refer the reader to specialized treatises, as[6, 25, 52, 53, 58, 66], where different notations are adopted. We like to refer also to the 1986 pa per by Schneider[55], where he first provided the Fox $H$-function representation of the stable distributions (with $\alpha \neq 1$) and to the 1990 book by Takayasu[56], where he first gave the diamond representation in the plane $\{\alpha, \theta\}$.

3 The Space-Time Fractional Diffusion

We now consider the Cauchy problem for the (spatially one-dimensional) space-time fractional diffusion (STFD) equation.

$$t D_\beta^\ast u(x,t) = x D_\theta^\alpha u(x,t), \quad u(x,0) = \delta(x), \quad x \in \mathbb{R}, \quad t \geq 0,$$

(3.1)

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

$$0 < \alpha \leq 2, \quad |\theta| \leq \min\{\alpha, 2 - \alpha\}, \quad 0 < \beta \leq 1.$$

(3.2)

Here $x D_\theta^\alpha$ denotes the Riesz-Feller fractional derivative of order $\alpha$ and skewness $\theta$, acting on the space variable $x$, and $t D_\beta^\ast$ denotes the Caputo fractional derivative of order $\beta$, acting on the time variable $t$. We recall the definitions of these fractional derivatives based on their representation in the Fourier and Laplace transform domain, respectively. So doing we avoid the subtleties lying in the inversion of the corresponding fractional integrals, see e.g. the 2001 survey by Mainardi et al.[29]. For general information on fractional integrals and derivatives we recommend the books[26, 48, 51].

3.1 The Riesz-Feller space-fractional derivative

We define the Riesz-Feller derivative as the pseudo-differential operator whose symbol is the logarithm of the characteristic function of a general Lévy strictly stable probability density with index of stability $\alpha$ and asymmetry parameter $\theta$ (improperly called skewness). As a consequence of Eq. (2.31), for a sufficiently well-behaved function $f(x)$, we define the Riesz-Feller space-fractional derivative of order $\alpha$ and skewness $\theta$ via the Fourier transform

$$\mathcal{F}\{x D_\theta^\alpha f(x); \kappa\} = -\psi_\alpha^\theta(\kappa) \hat{f}(\kappa), \quad \psi_\alpha^\theta(\kappa) = |\kappa|^{\alpha i \theta \text{sign} \kappa},$$

(3.3)
Notice that $i^{\theta} \text{sign} \kappa = \exp [i \text{sign} \kappa \theta \pi/2]$. For $\theta = 0$ we have a symmetric operator with respect to $x$, which can be interpreted as

$$x D_0^\alpha = - \left( -\frac{d^2}{dx^2} \right)^{\alpha/2},$$  \hspace{1cm} (3.4)$$
as can be formally deduced by writing $-|\kappa|^\alpha = -(\kappa^2)^{\alpha/2}$. We thus recognize that the operator $D_0^\alpha$ is related to a power of the positive definitive operator $-\partial^2 = -\frac{d^2}{dx^2}$ and must not be confused with a power of the first order differential operator $\partial = \frac{d}{dx}$ for which the symbol is $-i\kappa$. An alternative illuminating notation for the symmetric fractional derivative is due to Zaslavsky [50], and reads

$$x D_0^\alpha = \frac{d^\alpha}{dx^\alpha}.$$  \hspace{1cm} (3.5)$$
For $0 < \alpha < 2$ and $|\theta| \leq \min \{\alpha, 2 - \alpha\}$ the Riesz-Feller derivative reads

$$x D_\theta^\alpha f(x) = \frac{\Gamma(1+\alpha)}{\pi} \left\{ \sin [(\alpha+\theta)\pi/2] \int_0^\infty \frac{f(x+\xi)-f(x)}{\xi^{1+\alpha}} d\xi + \sin [(\alpha-\theta)\pi/2] \int_0^\infty \frac{f(x-\xi)-f(x)}{\xi^{1+\alpha}} d\xi \right\}.$$  \hspace{1cm} (3.6)$$

### 3.2 The Caputo fractional derivative

For a sufficiently well-behaved function $f(t)$ we define the Caputo time-fractional derivative of order $\beta$ with $0 < \beta \leq 1$ through its Laplace transform

$$\mathcal{L} \{t D_\beta^\beta f(t); s\} = s^\beta \tilde{f}(s) - s^{\beta-1} f(0^+), \hspace{0.5cm} 0 < \beta \leq 1.$$  \hspace{1cm} (3.7)$$
This leads us to define

$$t D_\beta^\beta f(t) := \begin{cases} \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{f^{(1)}(\tau)}{(t-\tau)^\beta} d\tau, & 0 < \beta < 1, \\
\frac{d}{dt} f(t), & \beta = 1. \end{cases}$$  \hspace{1cm} (3.8)$$
For the essential properties of the Caputo derivative, see [4, 13, 48].
3.3 The fundamental solution of the space-time fractional diffusion equation

Let us note that the solution \( u(x,t) \) of the Cauchy problem (3.1)–(3.2), 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 \( \sigma^2 = 2t \). Sometimes, to point out the parameters, we may denote the fundamental solution as

\[
    u(x,t) = G_{\alpha,\beta}(x,t) ,
\]

For our purposes let us here confine ourselves to recall the representation in the Laplace-Fourier domain of the (fundamental) solution as it results from the application of the transforms of Laplace and Fourier to Eq. (3.1). Using \( \hat{\delta}(\kappa) \equiv 1 \) we have:

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

hence

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

For explicit expressions and plots of the fundamental solution of (3.1) in the space-time domain we refer the reader to Mainardi, Luchko and Pagnini[29]. There, starting from the fact that the Fourier transform of the fundamental solution can be written as a Mittag-Leffler function with complex argument,

\[
    \hat{u}(\kappa,t) = \hat{G}_{\alpha,\beta}(\kappa,t) = E_{\beta} \left( -|\kappa|^{\alpha} i^{\beta} \text{sign} \kappa t^{\beta} \right) ,
\]

these authors have derived a Mellin-Barnes integral representation of \( u(x,t) = G_{\alpha,\beta}(x,t) \) with which they have proved the non-negativity of the solution for values of the parameters \( \{\alpha, \theta, \beta\} \) in the range (3.2) and analyzed the evolution in time of its moments. The representation of \( u(x,t) \) in terms of Fox \( H \)-functions can be found in Mainardi, Pagnini and Saxena[31], see also Chapter 6 in the recent book by Mathai, Saxena and Haubold[34].

We note, however, that the solution of the STFD Equation (3.1) and its variants has been investigated by several authors; let us only mention some
of them [1, 2, 8, 9, 21, 22, 23, 35, 36, 38, 40, 41, 42, 43, 44, 49, 54], where the connection with the CTRW was also pointed out.

In particular the fundamental solution for the space fractional diffusion \( \{0 < \alpha < 2, \beta = 1\} \) is expressed in terms of a stable density of order \( \alpha \) and skewness \( \theta \),

\[
G^0_{\alpha,1}(x, t) = t^{-1/\alpha} L^\theta_{\alpha}(x/t^{1/\alpha}), \quad -\infty < x < +\infty, \quad t \geq 0. \tag{3.12}
\]

whereas for the time fractional diffusion \( \{\alpha = 2, 0 < \beta < 1\} \) in terms of a (symmetric) M-Wright function of order \( \beta/2 \),

\[
G^0_{2,\beta}(x, t) = \frac{1}{2} t^{-\beta/2} M_{\beta/2}(|x|/t^{\beta/2}), \quad -\infty < x < +\infty, \quad t \geq 0. \tag{3.13}
\]

For the standard diffusion \( \{\alpha = 2, \beta = 1\} \) we recover the Gaussian density

\[
G^0_{2,1}(x, t) = \frac{1}{2\sqrt{\pi t}} e^{-x^2/(4t)} = t^{-1/2} L^0_2(x/t^{1/2}) = \frac{1}{2} t^{-1/2} M_{1/2}(|x|/t^{1/2}).
\]

Let us finally recall that the M-Wright function does appear also in the fundamental solution of the rightward time fractional drift equation,

\[
_{t}D^\beta u(x, t) = -\frac{\partial}{\partial x} u(x, t), \quad -\infty < x < +\infty, \quad t \geq 0. \tag{3.14}
\]

Denoting by \( G^*_{\beta}(x, t) \) this fundamental solution, we have

\[
G^*_{\beta}(x, t) = \left\{ \begin{array}{ll}
t^{-\beta} M_\beta \left( \frac{x}{t^\beta} \right), & x > 0, \\
0, & x < 0,
\end{array} \right. \tag{3.15}
\]

that for \( \beta = 1 \) reduces to the right running pulse \( \delta(x - t) \) for \( x > 0 \). For details see [15, 30].

### 3.4 Alternative forms of the space-time fractional diffusion equation

We note that in the literature there exist other forms alternative and equivalent to Eq. (3.1) with initial condition \( u(x, 0) = u_0(x) \) including the case \( u_0(x) = \delta(x) \). For this purpose we must briefly recall the definitions of fractional integral and fractional derivative according to Riemann-Liouville.
The Riemann-Liouville fractional integral for a sufficiently well behaved function \( f(t) \) \( (t \geq 0) \) is defined for any order \( \mu > 0 \) as

\[
\mathcal{I}^\mu f(t) := \frac{1}{\Gamma(\mu)} \int_0^t (t-\tau)^{\mu-1} f(\tau) \, d\tau.
\]

(3.16)

We note the convention \( \mathcal{I}^0 = I \) (Identity) and the semigroup property

\[
\mathcal{I}^\mu \mathcal{I}^\nu = \mathcal{I}^{\mu+\nu}, \quad \mu \geq 0, \nu \geq 0.
\]

(3.17)

The fractional derivative of order \( \mu > 0 \) in the Riemann-Liouville sense is defined as the operator \( \mathcal{D}^\mu \) which is the left inverse of the Riemann-Liouville integral of order \( \mu \) (in analogy with the ordinary derivative),

\[
\mathcal{D}^\mu \mathcal{I}^\mu = I, \quad \mu > 0.
\]

(3.18)

If \( m \) denote the positive integer such that such that \( m - 1 < \mu \leq m \), we recognize from Eqs. (3.16) – (3.18):

\[
\mathcal{D}^\mu f(t) := \mathcal{D}^m \mathcal{I}^{m-\mu} f(t).
\]

(3.19)

Then, restricting our attention to a order \( \beta \) with \( 0 < \beta \leq 1 \) (namely \( m = 1 \)) the corresponding Riemann-Liouville fractional derivative turns out

\[
\mathcal{D}^\beta f(t) = \begin{cases} 
\frac{d}{dt} \left[ \frac{1}{\Gamma(1-\beta)} \int_0^t \frac{f(\tau)}{(t-\tau)^\beta} \, d\tau \right], & 0 < \beta < 1, \\
\frac{d}{dt} f(t), & \beta = 1.
\end{cases}
\]

(3.20)

Then we get the relationship among the Caputo fractional derivative with the classical Riemann-Liouville fractional integral and derivative:

\[
\mathcal{D}^\beta f(t) := \mathcal{D}^1 \mathcal{I}^{1-\beta} f(t) = \mathcal{D}^\beta [f(t) - f(0)] = \mathcal{D}^\beta f(t) - \frac{f(0)}{\Gamma(1-\beta) t^{\beta}},
\]

(3.21)

and, as a consequence, the equivalence of (3.1) with the following problems

\[
u(x,t) = \mathcal{B} \mathcal{D}_x^\alpha \mathcal{I}_x^\beta u(x,t), \quad u(x,0) = \delta(x),
\]

(3.22)

\[
\frac{\partial}{\partial t} u(x,t) = \mathcal{D}_x^{1-\beta} \mathcal{D}_x^\alpha u(x,t), \quad u(x,0) = \delta(x).
\]

(3.23)
4 Analytic and stochastic pathways to subordination in space-time fractional diffusion

Our starting key-point to introduce the analytical and stochastic approaches to subordination in space-time fractional diffusion processes is the fundamental solution of the space-time fractional diffusion equation in the Laplace-Fourier domain given by (3.10).

4.1 The analytical interpretation via operational time.

Separating variables in (3.10) and using the trick to write \( \frac{1}{z + a} \) for \( \text{Re}(z + a) > 0 \) as a Laplace integral

\[
\frac{1}{z + a} = \int_{0}^{\infty} e^{-\rho z} e^{-a \rho} d\rho
\]

we have, identifying \( \rho := t_s \) as operational time, the following instructive expression for (3.10):

\[
\hat{u}(\kappa, s) = \int_{0}^{\infty} \left[ \exp \left( -t_s |\kappa|^{-\beta} \text{sign} \kappa \right) \right] \left[ s^{-1} \exp \left( -t_s s^{\beta} \right) \right] dt_s .
\]

(4.1)

We note that the first factor in (4.1)

\[
\hat{f}_{\alpha, \theta}(\kappa, t_s) := \exp \left( -t_s |\kappa|^{-\beta} \text{sign} \kappa \right)
\]

(4.2)

is the Fourier transform of a skewed stable density in \( x \), evolving in operational time \( t_s \), of a process \( x = y(t_s) \) along the real axis \( x \) happening in operational time \( t_s \), that we write as

\[
f_{\alpha, \theta}(x, t_s) = t_s^{-1/\alpha} L_{\alpha}^{\theta} \left( x/t_s^{1/\alpha} \right) .
\]

(4.3)

We can interpret the second factor

\[
\hat{q}_{\beta}(t_s, s) := s^{-1} \exp \left( -t_s s^{\beta} \right)
\]

(4.4)

as Laplace representation of the probability density in \( t_s \) evolving in \( t \) of a process \( t_s = t_s(t) \), generating the operational time \( t_s \) from the physical time \( t \), that is expressed via a fractional integral of a skewed Lévy density as

\[
q_{\beta}(t_s, t) = t_s^{-1/\beta} I_{1-\beta}^{t} L_{\beta}^{-\beta} \left( t/t_s^{1/\beta} \right) = t^{-\beta} M_{\beta}(t_s/t^{\beta}) ,
\]

(4.5)
see Eq. (2.26). To prove that \( q_\beta(t_*, t) \) (surely positive for \( t_* > 0 \)) is indeed a probability density we must further prove that is normalized,
\[
\int_{t_*=0}^{\infty} q_\beta(t_*, t) \, dt_*= 1.
\]
For this purpose it is sufficient to prove that its Laplace transform with respect to \( t_* \) is equal to 1 for \( s_* = 0 \). To get this Laplace transform \( \tilde{q}_\beta(s_*, t) \) we proceed as follows. Starting from the known Laplace transform with respect to \( t_* \),
\[
\tilde{q}_\beta(t_*, s) = s^{\beta-1} \exp \left( -t_* s^\beta \right),
\]
we apply a second Laplace transformation with respect to \( t_* \) with parameter \( s_* \) to get
\[
\tilde{\tilde{q}}_\beta(s_*, s) = \frac{s^{\beta-1}}{s_* + s^\beta},
\]
so, by inversion with respect to \( t_* \)
\[
\tilde{q}_\beta(s_*, t) = \int_{t_*=0}^{\infty} e^{-s_* t} \tilde{q}_\beta(t_*, t) \, dt_* = E_\beta(-s_* t^\beta),
\]
and setting \( s_* = 0 \)
\[
\int_{t_*=0}^{\infty} q_\beta(t_*, t) \, dt_* = E_\beta(0) = 1.
\]
Weighting the density of \( x = y(t_*) \) with the density of \( t_* = t_*(t) \) over \( 0 \leq t < \infty \) yields the density \( u(x, t) \) in \( x \) evolving with time \( t \).

In physical variables \( \{x, t\} \), using Eqs. (4.1) – (4.5), we have the subordination integral formula
\[
u(x, t) = \int_{t_*=0}^{\infty} f_{\alpha, \theta}(x, t_*) \, q_\beta(t_*, t) \, dt_*,
\]
where \( f_{\alpha, \theta}(x, t_*) \) (density in \( x \) evolving in \( t_* \)) refers to the process \( x = y(t_*) \) \( (t_* \to x) \) generating in “operational time” \( t_* \) the spatial position \( x \), and \( q_\beta(t_*, t) \) (density in \( t_* \) evolving in \( t \)) refers to the process \( t_* = t_*(t) \) \( (t \to t_*) \) generating from physical time \( t \) the “operational time” \( t_* \).

Our aim is to construct a process \( x = x(t) \) whose probability density is \( u(x, t) \), density in \( x \), evolving in \( t \). We will soon find justification for denoting the variable of integration by \( t_* \). We will exhibit it as the “operational time” for our fractional diffusion process, and for distinction we will call the variable \( t \) its “physical time” In fact \( f_{\alpha, \theta}(x, t_*) \) is a probability density in \( x \in \mathbb{R} \), evolving in operational time \( t_* > 0 \) and \( q_\beta(t_*, t) \) is a probability density in \( t_* \geq 0 \), evolving in physical time \( t > 0 \).
4.2 Stochastic interpretation.

Clearly $f_{\alpha,\theta}(x, t_*)$ characterizes a stochastic process describing a trajectory $x = y(t_*)$ in the $(t_*, x)$ plane, that can be visualized as a particle travelling along space $x$, as operational time $t_*$ is proceeding. Is there also a process $t_* = t_*(t)$, a particle moving along the positive $t_*$ axis, happening in physical time $t$? Naturally we want $t_*(t)$ increasing, at least in the weak sense,

$$ t_2 > t_1 \implies t_*(t_2) \geq t_*(t_1) . $$

We answer this question in the affirmative by showing that, by inverting the stable process $t = t(t_*)$ whose probability density (in $t$, evolving in operational time $t_*$) is the extremely positively skewed stable density

$$ r_{\beta}(t, t_*) = t_*^{-1/\beta} L^{-\beta}_t(t/t_*^{1/\beta}) . \quad (4.11) $$

In fact, recalling

$$ \tilde{r}_{\beta}(s, t_*) = \exp (-t_* s^\beta) , \quad (4.12) $$

there exists the stable process $t = t(t_*)$, weakly increasing, with density in $t$ evolving in $t_*$ given by (4.11). We call this process the leading process.

Happily, we can invert this process. Inversion of a weakly increasing trajectory means that horizontal segments are converted to vertical segments and vice versa jumps (as vertical segments) to horizontal segments (in graphical visualization).

Consider a fixed sample trajectory $t = t(t_*)$ and its also fixed inversion $t_* = t_*(t)$. Fix an instant $T$ of physical time and an instant $T_*$ of operational time. Then, because $t = t(t_*)$ is increasing, we have the equivalence

$$ t_*(T) \leq T_* \iff T \leq t(T_*) , $$

which, with notation slightly changed by

$$ t_*(T) \to t'_*, \ t_* \to t_*, \ T \to t , \ t(T_*) \to t'_* , $$

implies

$$ \int_0^{t_*} q(t'_*, t) \, dt'_* = \int_t^{\infty} r_{\beta}(t', t_*) \, dt' , \quad (4.13) $$

for the probability density $q(t_*, t)$ in $t_*$ evolving in $t$. It follows

$$ q(t_*, t) = \frac{\partial}{\partial t_*} \int_t^{\infty} r_{\beta}(t', t_*) \, dt' = \int_t^{\infty} \frac{\partial}{\partial t_*} r_{\beta}(t', t_*) \, dt' . $$
We continue in the $s_*$-Laplace domain assuming $t > 0$,

$$
\tilde{q}(s_*, t) = \int_t^\infty (s_* \tilde{r}_\beta(t', s_*) - \delta(t')) dt'.
$$

It suffices to consider $t > 0$, so that we have $\delta(t') = 0$ in this integral. Observing from (4.12)

$$
\tilde{r}_\beta(s, s) = \frac{1}{s + s^\beta},
$$

we find

$$
\tilde{r}_\beta(t, s_*) = \beta t^{-1} E_\beta(-s_* t^\beta),
$$

so that

$$
\tilde{q}(s_*, t) = \int_t^\infty s_* \beta t^\beta - 1 E_\beta(-s_* t^\beta) dt' = E_\beta(-s_* t^\beta),
$$

finally

$$
q(t_*, t) = t^{-\beta} M_\beta(t_*/t^\beta),
$$

From (4.16) we also see that

$$
\tilde{q}(s_*, s) = \frac{s^{\beta-1}}{s_* + s^\beta} = \tilde{q}_\beta(s_*, s),
$$

implying (4.6) and, see (4.7),

$$
q(t_*, t) \equiv q_\beta(t_*, t),
$$

so that indeed the process $t_* = t_*(t)$ is the inverse to the stable process $t = t(t_*)$ and has density $q_\beta(t_*, t)$.

**Remark.** The process at hand, $t_* = t_*(t)$, which is referred to as the inverse stable subordinator, is honoured with the name “Mittag-Leffler process” by Meerschaert at al. [35, 37]. Honouring this process by the name of Mittag-Leffler can be justified by the fact that by (4.16) the Laplace transform of its density is a Mittag-Leffler type function or by the fact that it is a properly scaled diffusion limit of the counting function $N(t)$ of the fractional generalization of the Poisson process whose residual waiting time probability is the Mittag-Leffler type function $E_\beta(-t^\beta)$, see recent papers of ours [11, 15]. In view of its probability density it may also be called the M-Wright process.

Stipulating that there exists a weakly increasing process $t_* = t_*(t)$ with density $q_\beta(t_*, t)$ we can analogously find the density of its inverse $t = t(t_*)$.
which comes just as \( r_\beta(t, t_*) \). However, in the context of our here presented considerations not being allowed to know that such process \( t_* = t_*(t) \) exists, we have taken as a gift from God the process \( t = t(t_*) \) and shown by its inversion that there exists a process \( t_* = t_*(t) \) with the desired properties.

From the density \( r_\beta(t, t_*) \) of the leading process \( t = t(t_*) \) we have found the density of the directing process \( t_* = t_*(t) \) as given by the Laplace transform pair (4.6), that is

\[
q_\beta(t_*, t) \div \tilde{q}_\beta(t_*, s) = s^{\beta-1} \exp(-t_*s^\beta).
\]

In physical coordinates we have (4.5) and (4.17), so also an expression through an \( M \)-Wright function,

\[
q_\beta(t_*, t) = t \int_0^\infty r_\beta(t, t_*) = t^{-\beta} M_\beta(t_*^\beta/t^\beta), \tag{4.20}
\]

see Eq. (2.26).

### 4.3 Evolution equations for the densities \( r_\beta(t, t_*) \) of \( t = t(t_*) \) and \( q_\beta(t_*, t) \) of \( t_* = t_*(t) \).

The Laplace-Laplace representation of the density \( r_\beta(t, t_*) \) of the process \( t = t(t_*) \) is, according to (4.14),

\[
\tilde{r}_\beta(s, s_*) = \frac{1}{s^{\beta} + s_*}.
\]

This implies

\[
s_* \tilde{r}_\beta(s, s_*) - 1 = -s^{\beta} \tilde{r}_\beta(s, s_*),
\]

and by inverting the transforms and observing the initial condition \( r_\beta(t, t_* = 0) = \delta(t) \) we arrive at the Cauchy problem

\[
\frac{\partial}{\partial t_*} r_\beta(t, t_*) = -t D_\beta^3 r_\beta(t, t_*), \quad r_\beta(t, t_* = 0) = \delta(t). \tag{4.21}
\]

Because it suffices to consider only \( t > 0 \) where \( \delta(t) = 0 \), we need not introduce a singular term on the right-hand side.

The Laplace-Laplace representation of the density \( q_\beta(t_*, t) \) of the process \( t_* = t_*(t) \) is, according to (4.18),

\[
\tilde{q}_\beta(s_*, s) = \frac{s^{\beta-1}_*}{s_* + s^\beta}.
\]
This implies
\[ s^\beta \tilde{q}_\beta(s_*, s) - s^\beta - 1 = -s_* \tilde{q}_\beta(s_*, s), \]
and by inverting the transforms and observing the initial condition \( q_\beta(t_*, t = 0) = \delta(t_*) \) we arrive at the Cauchy problem
\[ tD^\beta x(t, t_*) = -\frac{\partial}{\partial t_*} q_\beta(t_*, t) \quad q_\beta(t_*, t = 0) = \delta(t_*). \quad (4.22) \]
Because it suffices to consider only \( t_* > 0 \) where \( \delta(t_*) = 0 \), we can ignore the delta function on the right-hand side.

**Remark** The fractional differential equations in the above Cauchy problems have the same form. By replacing \( t \) by \( t_* \) and \( r \) by \( q \) one of them goes over into the other. However, in the first problem the delta initial condition refers to the fractional derivative (of order \( \beta \)), in the second problem to the ordinary (first order) derivative. These equations are akin with the time-fractional drift equation treated in (3.14) and (3.15), with different coordinates and proper initial conditions, as explained above. The process \( t = t(t_*) \) of the first problem is a positive-oriented (extreme) stable process, whereas the process \( t_* = t_*(t) \) is a fractional drift process, see (3.14)-(3.15) with \( x \) replaced by \( t_* \). The reason for the two evolution equations to have the same form is that the described two processes are inverse to each other, their graphical representations coincide just by interchanging the coordinate axes. The delta initial condition for each equation is given at value zero of the evolution variable for the variable in which the solution is a density.

### 4.4 The random walks.

We can now construct the process \( x = x(t) \) for the position \( x \) of the particle depending on physical time \( t \) as follows in two ways. With the variable \( t \) (physical time), \( t_* \) (operational time), \( x \) (position), we have the processes (i), (ii) and (iii), as follows:

(i) \( t = t(t_*) \) with density \( r_\beta(t, t_*) \) in \( t \), evolving in \( t_* \), the leading process,
(ii) \( x = y(t_*) \) with density \( f_{\alpha,\beta}(x, t_*) \) in \( x \), evolving in \( t_* \), the parent process,
(iii) \( t_* = t_*(t) \) with density \( q_\beta(t_*, t) \) in \( t_* \), evolving in \( t \), the directing process.

Observing that the processes (i) and (iii) are inverse to each other, and taking account of the subordination integral (4.10), we define the space-time fractional diffusion process as the subordinated process
\[ x = x(t) = y(t_*(t)). \quad (4.23) \]
Simulation of a trajectory for the subordinated process means: generate in running physical time \( t \) the operational time \( t_* \), then the operational process \( y(t_*) \).

Now, the Mittag-Leffler (or M-Wright) process \( t_*=t_*(t) \) is non-Markovian and not so easy to simulate. The alternative (we call it ”parametric subordination”) is to produce in dependence of the operational time \( t_* \) the processes (i) and (ii) and then eliminate \( t_* \) from the system

\[ t = t(t_*), \quad x = y(t_*), \tag{4.24} \]

to get \( x = x(t) \) from \( x = y(t_*) \) by change of time from \( t_* \) to \( t \).

We can produce a sequence of precise snapshots of \( t = t(t_*) \) and \( x = y(t_*) \) in the \((t_*,t)\) plane and the \((t_*,x)\) plane by setting, with a step-size \( \tau_* > 0 \),

\[ t_{*,n} = n\tau_*, \quad \bar{t}_n = T_{*,1} + T_{*,2} + \cdots + T_{*,n}, \quad \bar{x}_n = X_{*,1} + X_{*,2} + \cdots + X_{*,n}, \tag{4.25} \]

taking for \( k = 1,2,\ldots,n \) each \( T_{*,k} \) as a random number with density \( \tau_*^{-1/\beta} L^{-\beta}(t/\tau_*^{1/\beta}) \) and each \( X_{*,k} \) as a random number with density \( \tau_*^{-1/\alpha} L^{\theta}(x/\tau_*^{1/\alpha}) \), corresponding by self-similarity to the step \( \tau_* \).

We can do this by taking random numbers \( T_k \) and \( X_k \) with density \( L^{-\beta}(t) \) and \( L^{\theta}(x) \), respectively, and then with \( \tau = \tau_*^{1/\beta} \) and \( h = \tau_*^{1/\alpha} \), setting \( T_{*,k} = \tau T_k, \quad X_{*,k} = h X_k \). In other words: we produce (a renewal process at equidistant times with reward) a positively oriented random walk on the half-line \( t \geq 0 \) and a random walk on \(-\infty < x < +\infty \) with jumps at equidistant operational time instants \( t_* = n\tau_* \). We recognize the scaling relation \( \tau_*^{\beta}/h^{\alpha} \equiv 1 \), analogous to that used by us in earlier papers of ours on well-scaled passage to the diffusion limit in CTRW under power law regime, see [12, 15, 16]. Methods for producing stable random deviates can be found in the books [24, 25].

Finally, we transfer into the \((t,x)\) plane the points with coordinates \( \bar{t}_n, \bar{x}_n = \bar{y}_n \) and so obtain a sequence of precise snapshots of a true process \( x = x(t) \). Finer details of the process \( x = x(t) \) become visible by using smaller values of the operational step-size \( \tau_* \).
5 Graphical representations and Conclusions

We recall that, denoting the physical time with $t$, the operational time with $t_*$, the physical space with $x$ the density of the fractional diffusion process turns out to be given by the following subordination integral, see (4.10),

$$u(x,t) = \int_{t_*=0}^{\infty} f_{\alpha,\theta}(x,t_*) q_\beta(t_*,t) \, dt_*\,, \quad (5.1)$$

where $f_{\alpha,\theta}(x,t_*)$ is the density (in $x$ evolving in $t_*$) of the parent process $x = y(t_*) = x(t(t_*))$ and $q_\beta(t_*,t)$ is the density (in $t_*$ evolving in $t$) of the directing process $t_* = t_*(t)$.

By using the Fourier-Laplace pathway we recall the two densities related to the parameters $\alpha, \theta, \beta$ from (4.3) – (4.5),

$$f_{\alpha,\theta}(x,t_*) = t_*^{-1/\alpha} L_{\alpha}^\theta \left( x/t_1^{1/\alpha} \right) , \quad (5.2)$$

$$q_\beta(t_*,t) = t_*^{-1/\beta} t^{1-\beta} L_{\beta}^{-\beta} \left( t/t_1^{1/\beta} \right) = t^{-\beta} M_{\beta}(t_*/t^{\beta}) , \quad (5.3)$$

where $L$ refers to the Lévy stable density and $M$ to the Wright function, both introduced in Section 2. But for the parametric subordination the relevant density is $r_\beta(t,t_*)$ governing the leading process, a density in the physical time $t$ evolving with the operational time $t_*$: it turns out to be the unilateral Lévy density of order $\beta$, namely, see (4.11),

$$r_\beta(t,t_*) = t_*^{-1/\beta} L_{\beta}^{-\beta} \left( t_*/t_1^{1/\beta} \right) . \quad (5.4)$$

We have shown in Section 4.4 that in our approach (referred to as parametric subordination) the process of space-time fractional diffusion (non-Markovian for $\beta < 1$) can be simulated by two Markovian processes governed by stable densities, provided by $f_{\alpha,\theta}(x,t_*)$ and $r_\beta(t,t_*)$, as pointed out in our 2007 paper with Vivoli[18], where we have dealt with the CTRW model. There, before passing to the diffusion limit, we have two Markov processes happening on a discrete set of equidistant instants (for simplicity the non-negative integers) $n = 0,1,2,\ldots$, meaning $\tau_* = 1$, one of them moving randomly rightwards along $t \geq 0$, the other moving randomly on the real line $-\infty < x < \infty$ with jumps $T_n$ and $X_n$, respectively, for $n \geq 1$. By summing the "waiting times" $T_k$ and the jumps $X_k$ from 1 to $n$ we obtain sequences of jump instants $t = t_n$ and positions $x = x_n$, that we display in the $(t,x)$ plane. In fact, CTRW is the virgin form of parametric subordination.
We note that our approach is akin to that based on two stochastic differential equations, known in Physics as Langevin equations, see [7, 27, 65]. We have indicated these two stochastic differential equations in [18]. Here now we content ourselves with referring to the above cited papers.

In Section 4.4 we have splitted the fractional diffusion process into three processes (i), (ii), (iii), each of them containing two of the three coordinates: space \( x \), physical time \( t \), operational time \( t_* \). We simulate the leading process by a random walk \((rw_1)\), the parent process by a random walk \((rw_2)\), and the subordinated process (which yields the desired trajectory) by a random walk \((rw)\). The inversion of \((rw_1)\) gives us a random walk \((rw_3)\) for simulation of the directing process \( t_* = t_*(t) \). Essentially, we need to carry out only \((rw_1)\) and \((rw_2)\) according to the equations (4.25). By transferring the points \((\bar{t}_n, \bar{x}_n)\) into the \((t,x)\) plane we get the random walk \((rw)\) as visualization of a random trajectory \( x = x(t) = y(t_*(t)) \) according to the subordinated process which is our space-time fractional diffusion process of interest.

To make transparent the situation we display as a diagram in Fig. 2 the connections between the four random walks. It is now instructive to show some numerical realizations of these random walks for two case studies of symmetric (\( \theta = 0 \)) fractional diffusion processes: \{\( \alpha = 2, \beta = 0.80 \}\}, \{\( \alpha = \}

![Figure 2: Diagram for the connections between the four random walks (\( rw_1 \), (\( rw_2 \), (\( rw_3 \) and (\( rw \), related to the leading, parent, directing and subordinated processes, respectively.](image)
As explained in a previous sub-section, for each case we need to construct the sample paths for three distinct processes, the leading process \( t = t(t_*) \), the parent process \( x = y(t_*) \) (both in the operational time) and, finally, the subordinated process \( x = x(t) \), corresponding to the required fractional diffusion process.

We shall depict the above sample paths in Figs. 3, 4, 5 respectively, devoting the left and the right plates to the different case studies.

Plots in Fig. 3 (devoted to the leading process, the limit of \( (rw_1) \)) thus represent sample paths in the \( (t_*, t) \) plane of unilateral Lévy motions of order \( \beta \). By interchanging the coordinate axes we can consider Fig. 3 as representing sample paths of the directing process, the limit of \( (rw_3) \).

Plots in Fig. 4 (devoted to the parent process, the limit of \( (rw_2) \)) represent sample paths in the \( (t_*, x) \) plane, produced in the way explained above, for Lévy motions of order \( \alpha \) and skewness \( \theta = 0 \) (symmetric stable distributions).

By the indicated method, see (4.25), we have with (for simplicity) \( \tau_* = 1 \), \( \theta = 0 \) (symmetry) produced 10000 numbers \( \tilde{t}_n \) and corresponding numbers \( \tilde{y}_n \). Plotting the points \((t_{n,*}, \tilde{t}_n)\) into the \((t_*, t)\) (operational time, physical time) plane, the points \((t_{n,*}, \tilde{y}_n)\) into the \((t_*, x)\) (operational time, position in space) plane we get Fig. 3 and Fig. 4 for visualization of \((rw_1)\) and \((rw_2)\), respectively. Fig. 5 (as a visualization of \(rw\)) is obtained by plotting the points \((\tilde{t}_n, \tilde{y}_n)\) into the \((t, x)\) (physical time and space) plane.

Actually, we have invested a little bit more work in producing the figures. Namely, to make visible the jumps as vertical segments, we have in Fig. 3 connected the points \((t_{n,*}, \tilde{t}_n)\) and \((t_{n,*+1}, \tilde{t}_n)\) by a horizontal segment, the points \((t_{n,*+1}, \tilde{t}_n)\) and \((t_{n,*+1}, \tilde{t}_{n+1})\) by a vertical segment. Analogously in Fig. 4 with the indexed \( \tilde{t} \) replaced by indexed \( \tilde{y} \). In Fig. 5 we have connected the points \((\tilde{t}_n, \tilde{y}_n)\) and \((\tilde{t}_{n+1}, \tilde{y}_n)\) by a horizontal segment, the points \((\tilde{t}_{n+1}, \tilde{y}_n)\) and \((\tilde{t}_{n+1}, \tilde{y}_{n+1})\) by a vertical segment.

Resuming, we can consider Fig. 3 as a representation of \((rw_1)\) for the leading process, or by interchange of axes as one of \((rw_3)\) for the directing process, Fig. 4 as one of \((rw_2)\) for the parent process, and finally Fig. 5 as a representation of \(rw\) for the subordinated process which is our space-time fractional diffusion process.
Figure 3: A sample path for \((rw_1)\), the leading process \(t = t(t_*)\).
LEFT: \(\{\alpha = 2, \beta = 0.80\}\), RIGHT: \(\{\alpha = 1.5, \beta = 0.90\}\).

Figure 4: A sample path for \((rw_2)\), the parent process \(x = y(t_*)\).
LEFT: \(\{\alpha = 2, \beta = 0.80\}\), RIGHT: \(\{\alpha = 1.5, \beta = 0.90\}\).

Figure 5: A sample path for \((rw)\), the subordinated process \(x = x(t)\).
LEFT: \(\{\alpha = 2, \beta = 0.80\}\), RIGHT: \(\{\alpha = 1.5, \beta = 0.90\}\).
Figure 6: 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 7: 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 8: 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 9: A sample path for the parent process $x = y(t_*)$.  
LEFT: $\{\alpha = 2, \ N = 10^1\}$, RIGHT: $\{\alpha = 1.5, \ N = 10^1\}$.

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

Figure 11: A sample path for the parent process $x = y(t_*)$.  
LEFT: $\{\alpha = 2, \ N = 10^3\}$, RIGHT: $\{\alpha = 1.5, \ N = 10^3\}$.  

32
Figure 12: A sample path for the subordinated process $x = x(t)$.
LEFT: $\{\alpha = 2, \beta = 0.80, N = 10^1\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.90, N = 10^1\}$.

Figure 13: A sample path for the subordinated process $x = x(t)$.
LEFT: $\{\alpha = 2, \beta = 0.80, N = 10^2\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.90, N = 10^2\}$.

Figure 14: A sample path for the subordinated process $x = x(t)$.
LEFT: $\{\alpha = 2, \beta = 0.80, N = 10^3\}$, RIGHT: $\{\alpha = 1.5, \beta = 0.90, N = 10^3\}$.  

33
We conclude by including additional Figures, showing the effect of taking smaller step-sizes $\tau^*$, equivalently larger values $N$ of steps following our analysis for the CTRW\[18\]. Figs.6,7,8, Figs.9,10,11, Figs.12,13,14 show the effect of making the operational step-length $\tau^*$ smaller or, equivalently, the number $N$ of operational steps larger for the sample paths of the leading, parent and subordinated processes, respectively. In these pictures $\tau^* = 1/N$, and we have taken $N = 10$, $N = 100$ and $N = 1000$. 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 $10^1$, $10^2$, $10^3$ of number of steps. As a matter of fact there is no visible difference in the transition for the successive decades $10^4$, $10^5$, $10^6$ of number of steps as the great majority of spatial jumps and waiting times even for very small steps $\tau^*$ of the operational time. This property also explains the visible persistence of large jumps and waiting times.

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