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Time-fractional Diffusion of Distributed Order

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Abstract: The partial differential equation of Gaussian diffusion is generalized by using the time-fractional derivative of distributed order between 0 and 1, in both the Riemann-Liouville and the Caputo sense. For a general distribution of time orders we provide the fundamental solution, which is a probability density, in terms of an integral of Laplace type. The kernel depends on the type of the assumed fractional derivative, except for the single order case where the two approaches turn out to be equivalent. We consider in some detail two cases of order distribution: Double-order, and uniformly distributed order. Plots of the corresponding fundamental solutions and their variance are provided for these cases, pointing out the remarkable difference between the two approaches for small and large times.

Key words: Anomalous diffusion, fractional derivatives, Mittag-Leffler function, Laplace transform, Fourier transform

1. INTRODUCTION

It is well known that the fundamental solution (or Green function) for the Cauchy problem of a linear diffusion equation can be interpreted as a Gaussian (normal) probability density function (*pdf*) in space, evolving in time. All the moments of this *pdf* are finite; in particular, its variance is proportional to the first power of time, a noteworthy property of the *standard diffusion*.

In this article we will illustrate two types of generalization of this Cauchy problem, using fractional calculus. One of these uses the fractional derivative in the sense of Riemann and Liouville (R-L), the other in the sense of Caputo (C). We will distinguish between single and distributed orders of fractional derivatives. Specifically, we work out how to express their fundamental solutions in terms of an integral of Laplace type suitable for numerical

evaluation. Particular attention is devoted to the time evolution of the variance for the R-L and C cases. It is known that for large times, the variance characterizes the type of anomalous diffusion.

The remainder of the article is arranged as follows: In Section 2 we provide the general forms of the time-fractional diffusion equation with distributed order for both R-L and C derivatives, and the Fourier-Laplace representation of the corresponding fundamental solution. For this purpose, we introduce a positive function $p(\beta)$, which acts as a discrete or continuous distribution of orders. In addition to the particular case of a single order β_0 with $0 < \beta_0 \leq 1$, we consider two case-studies for the fractional diffusion of distributed order: A discrete distribution with two distinct orders β_1 and β_2 ($0 < \beta_1 < \beta_2 \leq 1$), and a continuous distribution consisting of the uniform density of orders between zero and 1.

Section 3 is devoted to the time evolution of the variance, which is obtained from the Fourier-Laplace representation of the corresponding fundamental solution, by inverting the Laplace transform (only). In the single order case, we recover the sub-diffusion power-law common to the R-L and C forms; for the distributed order cases we find a remarkable difference between the two forms, clearly visible in their asymptotic expressions for small and large times. In section 4 we illustrate our method for determining the fundamental solutions from their Fourier-Laplace transforms, carrying out first the Fourier inversion and then the Laplace inversion. The graphical representation of the fundamental solutions (in space at fixed times) is instructive. For the case of fractional diffusion of single order, we limit ourselves, because of the self-similarity of the solutions, to plots of the corresponding solutions against x at a fixed time $t = 1$. For the two case-studies of fractional relaxation of distributed order, because the self-similarity of the solutions is lost, we provide plots of the corresponding solutions against x at three fixed times, selected as $t = 0.1$, $t = 1$ and $t = 10$, contrasting the different evolution of the R-L and C forms, over a moderate space-range. We note how the time evolution of the solution in the spatial range considered depends on the different time-asymptotic behaviour of the variance for the two forms.

Finally, concluding remarks are given in Section 5. Appendix A is devoted to the basic concepts of fractional calculus, while Appendices B and C deal with functions of the Mittag-Leffler and exponential integral types, respectively, in view of their relevance in our treatment.

2. EQUATIONS FOR TIME-FRACTIONAL DIFFUSION OF DISTRIBUTED ORDER

2.1. R-L and C Forms in the Space-time Domain

The standard diffusion equation, which reads (using re-scaled non-dimensional variables)

$$\frac{\partial}{\partial t} u(x, t) = \frac{\partial^2}{\partial x^2} u(x, t), \quad x \in \mathfrak{R}, \quad t \in \mathfrak{R}_0^+ \quad (1)$$

where $u(x, t)$ is the field variable, can be generalized by using the concept of a fractional derivative of distributed order in time. This concept first appeared in the work of Caputo (1969), and was later developed by Caputo himself, (Caputo, 1995, 2001) as well as by

Bagley and Torvik (Bagley and Torvik 2000a,b) A basic framework for the numerical solution of distributed-order differential equations has recently been introduced by Diethelm and colleagues (Diethelm and Ford, 2001; Diethelm and Luchko, 2004), and also by Hartley and Lorenzo (Lorenzo and Hartley, 2002; Hartley and Lorenzo, 2003).

For this purpose, we consider a function $p(\beta)$, which acts as a weight for the order of differentiation $\beta \in (0, 1]$ such that

$$p(\beta) \geq 0, \quad \text{and} \quad \int_0^1 p(\beta) d\beta = c > 0. \tag{2}$$

The positive constant c can be taken as 1 if we wish to assume the normalization condition for the integral. Clearly, some special conditions of regularity and behaviour near the boundaries will be required for the weight function $p(\beta)$. Specifically, we require, for convenience, that its primitive $P(\beta) = \int_0^\beta p(\beta') d\beta'$ vanishes at $\beta = 0$, and is continuous to that point from the right, attains the value c at $\beta = 1$ and has at most finitely many (upwards) jump points in the half-open interval $0 < \beta \leq 1$, these jump points allowing delta contributions to $p(\beta)$ (this last is particularly relevant for discrete distributions of orders). This function, which can be called the *order density* if $c = 1$, is allowed to have δ -components if we are interested in a discrete distribution of orders.

There are two possible forms of generalization, depending on whether we use fractional derivatives in the R-L or C sense. Correspondingly, we obtain the time-fractional diffusion equation of distributed order in the two forms:

$$\frac{\partial}{\partial t} u(x, t) = \int_0^1 p(\beta)_t D^{1-\beta} \left[\frac{\partial^2}{\partial x^2} u(x, t) \right] d\beta, \quad x \in \mathfrak{R}, t \geq 0 \tag{3}$$

and

$$\int_0^1 p(\beta) [{}_t D_*^\beta u_*(x, t)] d\beta = \frac{\partial^2}{\partial x^2} u_*(x, t), \quad x \in \mathfrak{R}, t \geq 0. \tag{4}$$

From now on we shall restrict our attention to the fundamental solutions of equations (3) and (4), so we assume from now on that these equations are subject to the initial condition $u(x, 0^+) = u_*(x, 0^+) = \delta(x)$. Since, for distributed order, the solution depends on the selected form (as we shall show hereafter), we now distinguish the two fractional equations and their fundamental solutions by giving the variable $u(x, t)$ in the Caputo case the subscript $*$, as is customary for the notation of the corresponding derivative.

Several authors have recently discussed diffusion equations of distributed order of both the C type (see, e.g., Caputo, 2001; Chechkin et al., 2002, 2003a,b; Naber, 2004; Sokolov et al., 2004) and the R-L form (see, e.g., Sokolov et al., 2004; Sokolov and Klafter, 2005; Langlands, 2006). In some articles the authors have referred to the C and R-L forms as the “normal” and “modified” forms (respectively) of the time-fractional diffusion equation of distributed order. A general overview of fractional pseudo-differential equations of distributed order can be found in the work of Umarov and Gorenflo (2005). For a discussion of their relationship with continuous random walk models, the reader is referred to the work of Gorenflo and Mainardi (2005).

2.2. R-L and C Forms in the Fourier-Laplace Domain

The fundamental solutions for the time-fractional diffusion equations (3) and (4) can be obtained by applying the Fourier and Laplace transforms to them, in that sequence. For the generic functions $v(x)$ and $w(t)$, we write these transforms as

$$\begin{aligned} \mathcal{F}\{v(x); \kappa\} &= \widehat{v}(\kappa) := \int_{-\infty}^{+\infty} e^{i\kappa x} v(x) dx \quad \kappa \in \Re \\ \mathcal{L}\{w(t); s\} &= \widetilde{w}(s) := \int_0^{+\infty} e^{-st} w(t) dt \quad s \in \mathbb{C}. \end{aligned} \tag{5}$$

In the Fourier-Laplace domain, our Cauchy problems, with $u(x, 0^+) = u_*(x, 0^+) = \delta(x)$, appear (after applying formulae for the Laplace transform appropriate to the R-L and C fractional derivatives – see equations ((67) and ((66) – and observing $\widehat{\delta}(\kappa) \equiv 1$ (see, e.g., Gelfand and Shilov, 1964)) appear in the two forms

$$s\widehat{u}(\kappa, s) - 1 = -\kappa^2 \left[\int_0^\infty p(\beta) s^{1-\beta} d\beta \right] \widehat{u}(\kappa, s) \tag{6}$$

$$\left[\int_0^\infty p(\beta) s^\beta d\beta \right] \widehat{u}(\kappa, s) - \int_0^\infty p(\beta) s^{\beta-1} d\beta = -\kappa^2 \widehat{u}(\kappa, s). \tag{7}$$

Introducing the relevant functions

$$A(s) = \int_0^1 p(\beta) s^{1-\beta} d\beta \tag{8}$$

and

$$B(s) = \int_0^1 p(\beta) s^\beta d\beta \tag{9}$$

we get the Fourier-Laplace representation of the corresponding fundamental solutions for the R-L and C cases as

$$\widehat{u}(\kappa, s) = \frac{1}{s + \kappa^2 A(s)} = \frac{1/A(s)}{\kappa^2 + s/A(s)} \tag{10}$$

and

$$\widehat{u}_*(\kappa, s) = \frac{B(s)/s}{\kappa^2 + B(s)}. \tag{11}$$

From equations (10) and (11) we can see that conversion between the R-L and the C forms can be carried out using the transformation

$$\{\text{C} : B(s)\} \iff \left\{ \text{R-L} : \frac{s}{A(s)} \right\}. \tag{12}$$

Note that in the particular case of time fractional diffusion of single order β_0 ($0 < \beta_0 \leq 1$) we have $p(\beta) = \delta(\beta - \beta_0)$ and, hence, in equation ((8) $A(s) = s^{1-\beta_0}$, and in equation ((9): $B(s) = s^{\beta_0}$, so that $B(s) \equiv s/A(s)$. Thus, equations (10) and (11) provide the same result

$$\widehat{u}(\kappa, s) \equiv \widehat{u}_*(\kappa, s) = \frac{s^{\beta_0-1}}{\kappa^2 + s_0^\beta}. \tag{13}$$

This is consistent with the well-known result that the two forms are equivalent for the single order case. However, for a generic order distribution, the Fourier-Laplace representations (10) and (11) are different, and the two forms produce different fundamental solutions in the space-time domain; these can be seen to be interrelated in some way, in view of transformation (12).

3. VARIANCE OF THE FUNDAMENTAL SOLUTIONS

3.1. General Considerations

Before trying to determine the fundamental solutions in the space-time domain to be obtained by a double inversion of the Fourier-Laplace transforms, it is worth outlining the expressions of their second moment (that is, the variance), since these can be derived from equations (10) and (11) through a single Laplace inversion, as will now be shown. We recall that the time evolution of the variance is relevant for classifying the type of diffusion.

Denoting, for the two forms,

$$\text{R-L} : \sigma^2(t) := \int_{-\infty}^{+\infty} x^2 u(x, t) dx \quad \text{C} : \sigma_*^2(t) := \int_{-\infty}^{+\infty} x^2 u_*(x, t) dx \tag{14}$$

we recognize that

$$\text{R-L} : \sigma^2(t) = -\frac{\partial^2}{\partial \kappa^2} \widehat{u}(\kappa = 0, t), \quad \text{C} : \sigma_*^2(t) = -\frac{\partial^2}{\partial \kappa^2} \widehat{u}_*(\kappa = 0, t). \tag{15}$$

As a consequence, we need to invert only Laplace transforms, taking into account the behaviour of the Fourier transform for κ near zero.

For the R-L case, we get (from equation (10))

$$\widehat{u}(\kappa, s) = \frac{1}{s} \left(1 - \kappa^2 \frac{A(s)}{s} + \dots \right) \tag{16}$$

and thus obtain

$$\widetilde{\sigma}^2(s) = -\frac{\partial^2}{\partial \kappa^2} \widehat{u}(\kappa = 0, s) = \frac{2A(s)}{s^2}. \tag{17}$$

For the C-case, we get (from equation (11))

$$\widehat{u}_*(\kappa, s) = \frac{1}{s} \left(1 - \kappa^2 \frac{1}{B(s)} + \dots \right) \tag{18}$$

and thus obtain

$$\widetilde{\sigma}_*^2(s) = -\frac{\partial^2}{\partial \kappa^2} \widehat{u}_*(\kappa = 0, s) = \frac{2}{sB(s)}. \tag{19}$$

Except for single order diffusion, where we recover the well-know result

$$\sigma^2(t) \equiv \sigma_*^2(t) = 2 \frac{t^{\beta_0}}{\Gamma(\beta_0 + 1)} 0 < \beta_0 \leq 1 \tag{20}$$

we expect the time evolution of the variance for a generic order distribution to depend substantially on the chosen (R-L or C) form.

We will now consider some typical choices for the weight function $p(\beta)$ that characterizes the time-fractional diffusion equations of distributed order (3) and (4). This will allow us to compare the results for the R-L and C forms.

3.2. Double Order Fractional Diffusion

First, we consider the choice

$$p(\beta) = p_1 \delta(\beta - \beta_1) + p_2 \delta(\beta - \beta_2), \quad 0 < \beta_1 < \beta_2 \leq 1 \tag{21}$$

where the constants p_1 and p_2 are both positive, conveniently restricted to the normalization condition $p_1 + p_2 = 1$.

For the R-L case we have

$$A(s) = p_1 s^{1-\beta_1} + p_2 s^{1-\beta_2} \tag{22}$$

and so, in combination with equation (17), we have

$$\widetilde{\sigma}^2(s) = 2p_1 s^{-(1+\beta_1)} + 2p_2 s^{-(1+\beta_2)} \tag{23}$$

and the Laplace inversion yields

$$\sigma^2(t) = 2p_1 \frac{t^{\beta_1}}{\Gamma(\beta_1 + 1)} + 2p_2 \frac{t^{\beta_2}}{\Gamma(\beta_2 + 1)} \sim \begin{cases} 2p_1 \frac{t^{\beta_1}}{\Gamma(1+\beta_1)}, & t \rightarrow 0^+ \\ 2p_2 \frac{t^{\beta_2}}{\Gamma(1+\beta_2)}, & t \rightarrow +\infty \end{cases} \tag{24}$$

(cf. Sokolov et al., 2004; Langlands, 2006).

Similarly, for the C case we have

$$B(s) = p_1 s^{\beta_1} + p_2 s^{\beta_2} \tag{25}$$

giving, in combination with equation (19),

$$\widetilde{\sigma}_*^2(s) = \frac{2}{p_1 s^{(1+\beta_1)} + p_2 s^{(1+\beta_2)}} \tag{26}$$

and the Laplace inversion yields

$$\sigma_*^2(t) = \frac{2}{p_2} t^{\beta_2} E_{\beta_2-\beta_1, \beta_2+1} \left(-\frac{p_1}{p_2} t^{\beta_2-\beta_1} \right) \sim \begin{cases} \frac{2}{p_2} \frac{t^{\beta_2}}{\Gamma(1+\beta_2)}, & t \rightarrow 0^+ \\ \frac{2}{p_1} \frac{t^{\beta_1}}{\Gamma(1+\beta_1)}, & t \rightarrow +\infty \end{cases} \tag{27}$$

(cf. Chechkin et al., 2002).

We can see that for the R-L case we have an explicit combination of two power laws: The smaller exponent (β_1) dominates for small times, whereas the larger exponent (β_2) dominates for large times. For the C case, we have a Mittag-Leffler function in two parameters, and thus we have a combination of two power laws only asymptotically for small and large times. Specifically, we get a behaviour that is opposite to that for the R-L case, and so for the C case the larger exponent (β_2) dominates for small times whereas the smaller exponent (β_1) dominates for large times.

We can derive the above asymptotic behaviours directly from the Laplace transforms (23) and (26) by applying the Tauberian theory for Laplace transforms. According to this theory, the asymptotic behaviour of a function $f(t)$ near $t = \infty$ and $t = 0$ may be (formally) obtained from the asymptotic behaviour of its Laplace transform $\widetilde{f}(s)$ for $s \rightarrow 0^+$ and for $s \rightarrow +\infty$, respectively. In fact, for the R-L case, we note that for $A(s)$ in equation (22) $s^{1-\beta_1}$ is negligibly small in comparison with $s^{1-\beta_2}$ for $s \rightarrow 0^+$, while $s^{1-\beta_2}$ is negligibly small in comparison to $s^{1-\beta_1}$ for $s \rightarrow +\infty$. Similarly for the C case, $B(s)$ in (25) s^{β_2} is negligibly small in comparison to s^{β_1} for $s \rightarrow 0^+$, and s^{β_1} is negligibly small in comparison s^{β_2} for $s \rightarrow +\infty$.

3.3. Fractional Diffusion of Uniformly Distributed Order

Next, we consider the choice

$$p(\beta) = 1, \quad 0 < \beta < 1. \tag{28}$$

For the R-L case we have

$$A(s) = s \int_0^1 s^{-\beta} d\beta = \frac{s-1}{\log s} \tag{29}$$

and so, in combination with equation (17), we get

$$\widetilde{\sigma}^2(s) = 2 \left[\frac{1}{s \log s} - \frac{1}{s^2 \log s} \right]. \tag{30}$$

Then, by inversion (see Appendix C, equations (91) and (92), we get

$$\sigma^2(t) = 2[v(t, 0) - v(t, 1)] \sim \begin{cases} 2/\log(1/t), & t \rightarrow 0 \\ 2t/\log t, & t \rightarrow \infty \end{cases} \tag{31}$$

where $v(t, a) := \int_0^\infty \frac{t^{a+\tau}}{\Gamma(a+\tau+1)} d\tau$, $a > -1$ denotes a special function, introduced in Appendix C along with its Laplace transform.

For the C case, we have

$$B(s) = \int_0^1 s^\beta d\beta = \frac{s-1}{\log s} \tag{32}$$

and so, in combination with equation (19), we have

$$\widetilde{\sigma}_*^2(s) = \frac{2 \log s}{s-1}. \tag{33}$$

Then, by inversion (see Appendix C, equations (87) and (90) (cf. Checkkin et al., 2002, equations (23) to (27))), we get

$$\sigma_*^2(t) = 2 [\log t + \gamma + e^t \mathcal{E}_1(t)] \sim \begin{cases} 2t \log(1/t), & t \rightarrow 0 \\ 2 \log(t), & t \rightarrow \infty \end{cases} \tag{34}$$

where $\mathcal{E}_1(t) := \int_t^\infty \frac{e^{-u}}{u} du = e^{-t} \int_0^\infty \frac{e^{-u}}{u+t} du$ denotes the exponential integral function recalled in Appendix C, and $\gamma = 0.57721\dots$ is the Euler-Mascheroni constant.

For the uniform distribution, we find it instructive to compare the time evolution of the variances for the R-L and C forms with that corresponding to a number of single orders. The top part of Figure 1 shows results for moderate times ($0 \leq t \leq 10$) using linear scales, while the lower part displays those for large times ($10^1 \leq t \leq 10^7$), using logarithmic scales.

4. EVALUATION OF THE FUNDAMENTAL SOLUTIONS

4.1. The Two Strategies

In order to determine the fundamental solutions $u(x, t)$ and $u_*(x, t)$ in the space-time domain, we can use either of two alternative strategies related to the order in carrying out the inversions of the Fourier and Laplace transforms in equations (10) and (11)

1. invert the Fourier transform, giving $\widetilde{u}(x, s)$, $\widetilde{u}_*(x, s)$, and then invert the remaining Laplace transform (S1)
2. invert the Laplace transform, giving $\widehat{u}(\kappa, t)$, $\widehat{u}_*(\kappa, t)$, and then invert the remaining Fourier transform (S2)

Before considering the general case of time-fractional diffusion of distributed order, we will briefly recall the determination of the fundamental solution $u(x, t)$ (common to both the R-L and C forms) for the single order case.

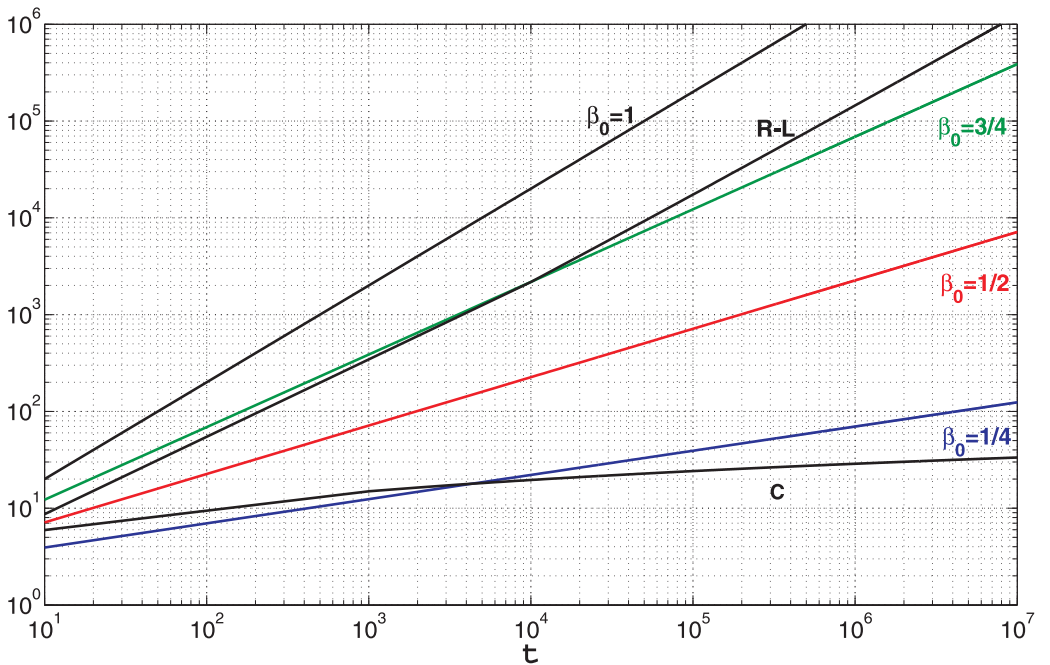
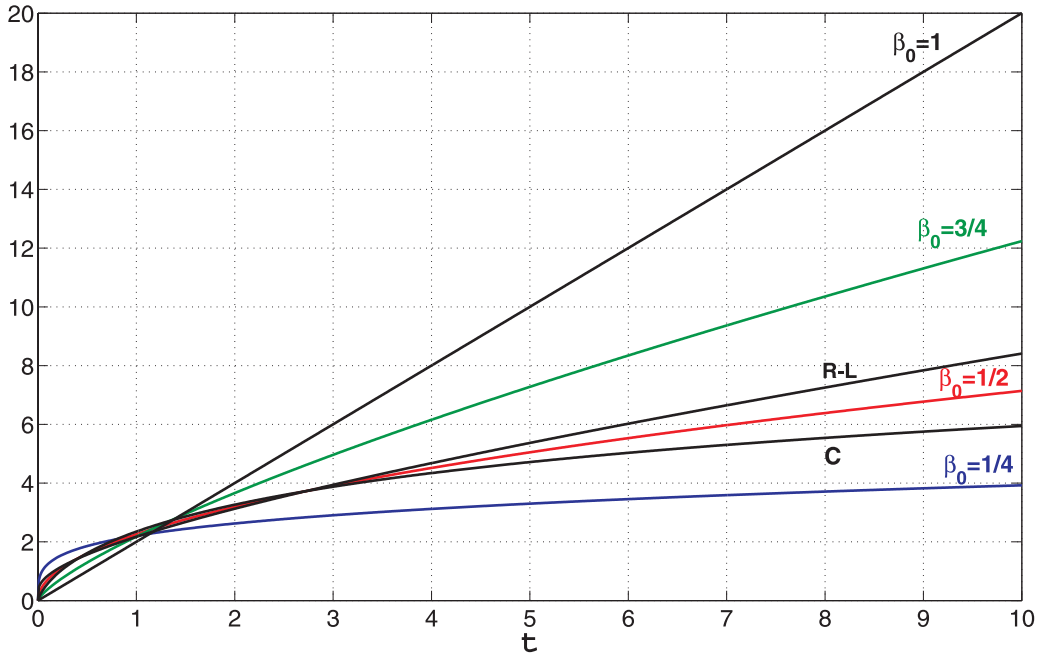


Figure 1. Variance against t for the uniform order distribution in both R-L and C forms, compared with a single order case. Top: $0 \leq t \leq 10$ (linear scales). Bottom: $10^1 \leq t \leq 10^7$ (logarithmic scales).

4.2. Single Order Diffusion

For the time-fractional diffusion equation of single order β_0 , strategy S1 yields the Laplace transform

$$\tilde{u}(x, s) = \frac{s^{\beta_0/2-1}}{2} e^{-|x|s^{\beta_0/2}}, \quad 0 < \beta_0 \leq 1. \tag{35}$$

This strategy was adopted by Mainardi (1993, 1996, 1997) to obtain the Green function in the form

$$u(x, t) = t^{-\beta_0/2} U(|x|/t^{\beta_0/2}), \quad -\infty < x < +\infty, \quad t \geq 0 \tag{36}$$

where the variable $X := x/t^{\beta_0/2}$ acts as a similarity variable and the function $U(x) := u(x, 1)$ denotes the reduced Green function. Restricting our attention to $x \geq 0$, the solution is

$$\begin{aligned} U(x) &= \frac{1}{2} M_{\beta_0/2}(x) = \frac{1}{2} \sum_{k=0}^{\infty} \frac{(-x)^k}{k! \Gamma[-\beta_0 k/2 + (1 - \beta_0/2)]} \\ &= \frac{1}{2\pi} \sum_{k=0}^{\infty} \frac{(-x)^k}{k!} \Gamma[\beta_0(k+1)/2] \sin[\pi \beta_0(k+1)/2] \end{aligned} \tag{37}$$

where $M_{\beta_0/2}(x)$ is an entire transcendental function (of order $1/(1 - \beta_0/2)$) of the Wright type (see Podlubny, 1999; Gorenflo et al., 1999, 2000b; Mainardi and Pagnini, 2003).

Since the fundamental solution has the property of self-similarity it is sufficient to consider the reduced Green function $U(x)$. Figure 2 shows the $U(x)$ for different orders ranging from $\beta_0 = 0$, for which we recover the Laplace density

$$U(x) = \frac{1}{2} e^{-|x|} \tag{38}$$

to $\beta_0 = 1$, for which we recover the Gaussian density (of variance $\sigma^2 = 2$)

$$U(x) = \frac{1}{2\sqrt{\pi}} e^{-x^2/4}. \tag{39}$$

Strategy S2 yields the Fourier transform

$$\hat{u}(\kappa, t) = E_{\beta_0}(-\kappa^2 t^{\beta_0}), \quad 0 < \beta_0 \leq 1 \tag{40}$$

where E_{β_0} denotes the Mittag-Leffler function (see Appendix B). The strategy (S2) has been used by Gorenflo et al. (2000a) and also by Mainardi et al. (2001, 2005) to obtain the Green functions of more general space-time-fractional diffusion equations (of single order), and requires us to invert the Fourier transform using the machinery of the Mellin convolution and the Mellin-Barnes integrals. Restricting ourselves here to recalling the final results, the

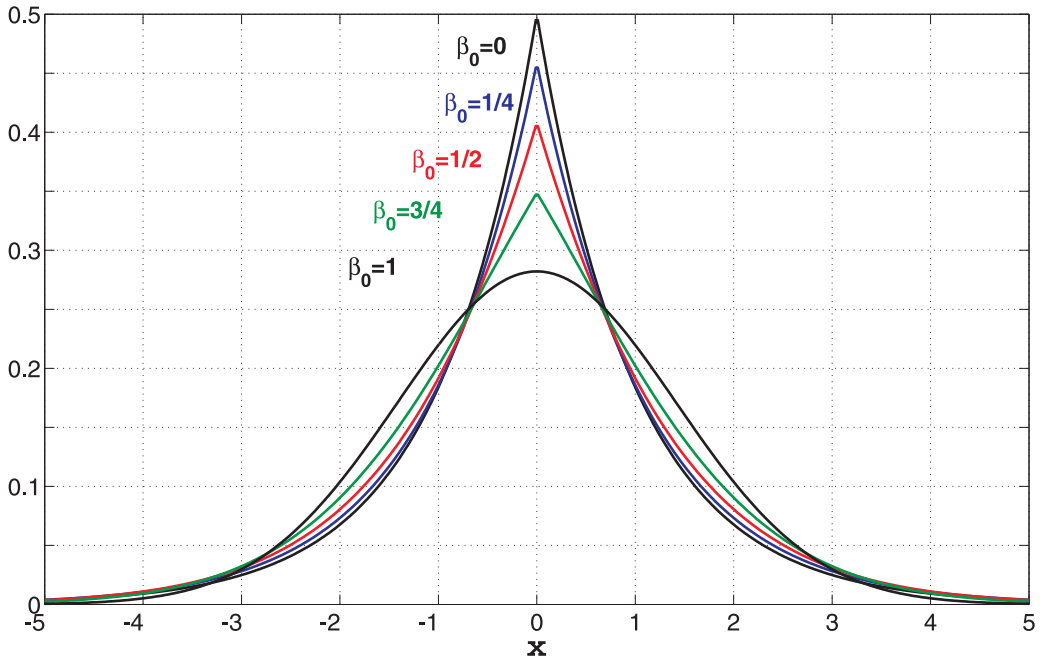


Figure 2. The reduced Green function $U(x) = \frac{1}{2}M_{\beta_0/2}(x)$ plotted against x , for the interval $|x| \leq 5$, with $\beta_0 = 0, 1/4, 1/2, 3/4, 1$.

reduced Green function for the time-fractional diffusion equation now appears, for $x \geq 0$, in the form

$$U(x) = \frac{1}{\pi} \int_0^\infty \cos(\kappa x) E_{\beta_0}(-\kappa^2) d\kappa = \frac{1}{2x} \frac{1}{2\pi i} \int_{\sigma-i\infty}^{\sigma+i\infty} \frac{\Gamma(1-s)}{\Gamma(1-\beta_0 s/2)} x^s ds \quad (41)$$

with $0 < \sigma < 1$. By solving the Mellin-Barnes integrals using the residue theorem, we arrive at the same power series of the M -Wright function as in the previous case (equation (37)).

Both strategies allow us to prove that the Green function is non-negative and normalized, and can thus be interpreted as a spatial probability density evolving in time, with similarity law (refeqno4.2). (For further discussion of the fundamental solutions of fractional diffusion equations of single order, see, e.g., Schneider and Wyss, 1989; Kochubei, 1990; Metzler et al., 1994; Saichev and Zaslavsky, 1997; Hilfer, 2000; Metzler and Klafter, 2000; Anh and Leonenko, 2001; Hanyga, 2002; Zaslavsky, 2002; Eidelman and Kochubei, 2004; and references therein).

4.3. Distributed Order Diffusion

As with single order diffusion, either strategy (S1) or strategy (S2) can be followed for cases of distributed order. In contrast with previous articles by our group, where we have followed the strategy S2 (Mainardi and Pagnini, 2006; Mainardi et al., 2006a,b), here we follow strat-

egy S1. This choice requires the Fourier transform pair (a straightforward exercise in complex analysis based on residue theorem and Jordan's lemma)

$$\frac{c}{d + \kappa^2} \xleftrightarrow{\mathcal{F}} \frac{c}{2d^{1/2}} e^{-|x|d^{1/2}}, \quad d > 0. \quad (42)$$

We can recognize, by comparing equation (42) with equations (10) and (11) that for the RL and C forms we have

$$\text{R-L : } \begin{cases} c = c(s) := 1/A(s) \\ d = d(s) := s/A(s) \end{cases} \quad \text{C : } \begin{cases} c = c(s) := B(s)/s \\ d = d(s) := B(s) \end{cases}. \quad (43)$$

Next, we invert the Laplace transforms obtained by substituting relevant parts of equation (43) into the right-hand side of equation (42).

For the R-L case we have

$$\tilde{u}(x, s) = \frac{1}{2[sA(s)]^{1/2}} \exp\{-|x|[s/A(s)]^{1/2}\} \quad (44)$$

while for the C case we have

$$\tilde{u}_*(x, s) = \frac{[B(s)]^{1/2}}{2s} \exp\{-|x|[B(s)]^{1/2}\}. \quad (45)$$

Following a standard procedure in complex analysis, the Laplace inversion requires integration along the borders of the negative real semi-axis in the s -complex cut plane. In fact, this semi-axis, defined by $s = re^{\pm i\pi}$ with $r > 0$, turns out to be the branch cut common for the functions $s^{1-\beta}$ (present in $A(s)$ for the R-L form) and s^β (present in $B(s)$ for the C form). Then, by means of the Titchmarsh theorem on Laplace inversion, we get the representations in terms of real integrals of Laplace type.

For the R-L case we get

$$u(x, t) = -\frac{1}{\pi} \int_0^\infty e^{-rt} \text{Im} \{ \tilde{u}(x, re^{i\pi}) \} dr \quad (46)$$

where, from equation (44), we must know $A(s)$ along the ray $s = re^{i\pi}$ with $r > 0$. We can thus write

$$A(re^{i\pi}) = \rho \cos(\pi\gamma) + i\rho \sin(\pi\gamma) \quad (47)$$

where

$$\begin{cases} \rho = \rho(r) = |A(re^{i\pi})| \\ \gamma = \gamma(r) = \frac{1}{\pi} \arg [A(re^{i\pi})] \end{cases}. \quad (48)$$

Similarly, for the C case we obtain

$$u_*(x, t) = -\frac{1}{\pi} \int_0^\infty e^{-rt} \operatorname{Im} \{ \tilde{u}_*(x, re^{i\pi}) \} dr \tag{49}$$

where, from equation (45), we must know $B(s)$ along the ray $s = re^{i\pi}$ with $r > 0$. We can thus write

$$B(re^{i\pi}) = \rho_* \cos(\pi \gamma_*) + i \rho_* \sin(\pi \gamma_*) \tag{50}$$

where

$$\begin{cases} \rho_* = \rho_*(r) = |B(re^{i\pi})| \\ \gamma_* = \gamma_*(r) = \frac{1}{\pi} \arg [B(re^{i\pi})] \end{cases} \tag{51}$$

As a consequence, we formally write the required fundamental solutions as

$$u(x, t) = \int_0^\infty e^{-rt} P(x, r) dr \quad P(x, r) = -\frac{1}{\pi} \operatorname{Im} \{ \tilde{u}(x, re^{i\pi}) \} \tag{52}$$

and

$$u_*(x, t) = \int_0^\infty e^{-rt} P_*(x, r) dr, \quad P_*(x, r) = -\frac{1}{\pi} \operatorname{Im} \{ \tilde{u}_*(x, re^{i\pi}) \} \tag{53}$$

where the functions $P(x, r)$ and $P_*(x, r)$ must be derived by using equations (44), (46), (47), (48) and (52), and equations (45), (49), (50), (51), and (53), respectively. We recognize that, in view of transformation (12), the expressions of P and P_* are related to each other by the transformation

$$\rho_*(r) \iff r/\rho(r), \quad \gamma_*(r) \iff 1 - \gamma(r). \tag{54}$$

We thus need only to provide the explicit expression for the C form:

$$\begin{aligned} P_*(x, r) &= \frac{1}{2\pi r} \operatorname{Im} \{ \rho_*^{1/2} e^{i\pi \gamma_*/2} \exp [-e^{i\pi \gamma_*/2} \rho_*^{1/2} x] \} \\ &= \frac{1}{2\pi r} \rho_*^{1/2} e^{-\rho_*^{1/2} x \cos(\pi \gamma_*/2)} \sin [\pi \gamma_*/2 - \rho_*^{1/2} x \sin(\pi \gamma_*/2)]. \end{aligned} \tag{55}$$

The corresponding expression of $P(x; r)$ for the R-L form can be obtained from equation (55) by applying transformation (54).

Note that the fundamental solutions found in this subsection are equivalent to those obtained by the current authors elsewhere (Mainardi et al., 2006a) by following strategy S2, after a lengthy manipulation of Mellin-Barnes integrals.

4.4. Plots of the Fundamental Solutions

Next, we exhibit some plots of the fundamental solutions for the two case studies considered in Section 3.2, in order to demonstrate the remarkable difference between the R-L and the C forms.

For the case with two orders, we use $\beta_1 = 1/4$ and $\beta_2 = 1$ to contrast the evolution of the fundamental solution for the R-L and the C forms.

Figure 3 shows plots of the R-L and C solutions plotted against x (in the interval $|x| \leq 5$), at times $t = 0.1$, $t = 1$, and $t = 10$. Within this limited spatial range we can see that the time evolution of the *pdf* depends on the different time-asymptotic behaviour of the variance for the two forms, as stated in equations (31) and (34).

For the uniform distribution, we find it instructive to compare, in Figure 4, the solutions corresponding to R-L and C forms with the solutions of the fractional diffusion of a single order $\beta_0 = 1/4$, $3/4$, and 1 at fixed times ($t = 1$, $t = 10$). ($\beta_0 = 1/2$ has been excluded to improve the clarity of the plots.)

5. CONCLUSIONS

We have investigated the time fractional diffusion equation with (discretely or continuously) distributed order between 0 and 1 in both the Riemann-Liouville and Caputo forms, providing the Fourier-Laplace representation of the corresponding fundamental solutions. For the case with only a single order, the two forms are equivalent, with a self-similar fundamental solution, but for a general order distribution the equivalence and the self-similarity are lost. In particular, the asymptotic behaviour of the fundamental solution and its variance at small and large times depends strongly on the approach selected. We have considered two simple but noteworthy case-studies of distributed order, namely the case of two different discrete orders β_1 and β_2 , and the case of a uniform order distribution.

In the first of these cases, one of the orders dominates the time-asymptotics near zero, and the other order dominates near infinity, but β_1 and β_2 change their roles when switching from the R-L form to the C form of the time-fractional diffusion. The asymptotics for uniform order density are remarkably different, the extreme orders now being (roughly speaking) 0 and 1. We now meet super-slow and slightly super-fast time behaviours of the variance as we approach zero and infinity, again with the R-L and C forms producing opposite behaviours to one another. The figures in Section 3.3, clearly show the effects mentioned (in particular, the extremely slow growth of the variance as $t \rightarrow \infty$ for the C form). After analysis of the variance, which in practice requires only the inversion of a Laplace transform, we considered the task of the double inversion of the Laplace-Fourier representation. For a general order distribution we were able to express the fundamental solution in terms of a Laplace integral in time with a kernel which depends on space and order distribution in a simple form, see equations (52) to (55). For the two case studies considered, the plots of the fundamental solutions (see Section 4.4) clearly show their dependence on the different asymptotic behavior of the corresponding variance.

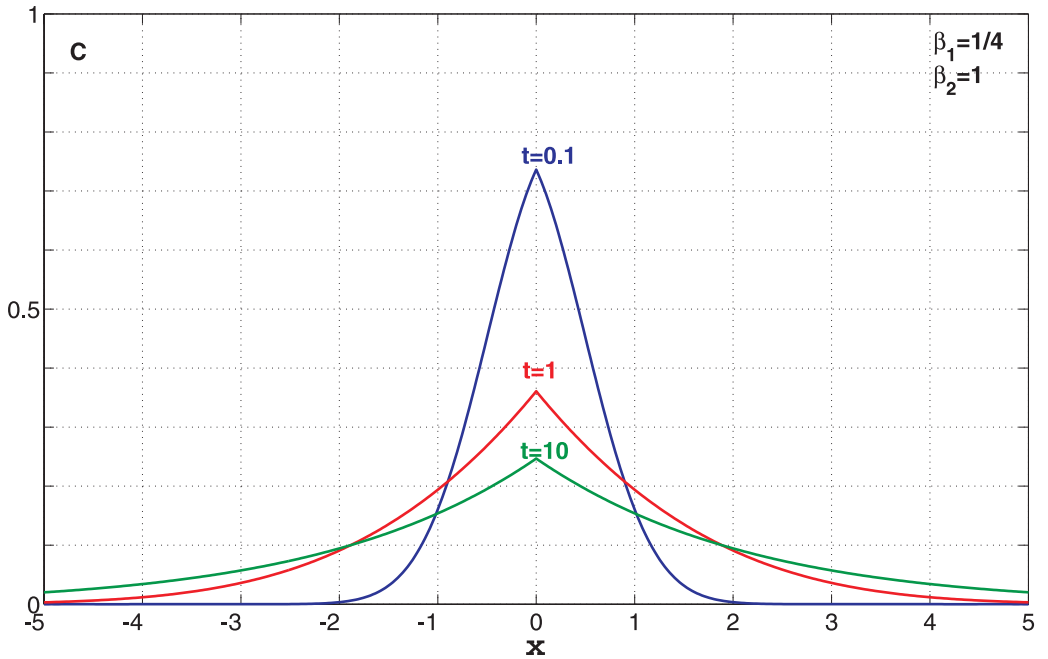
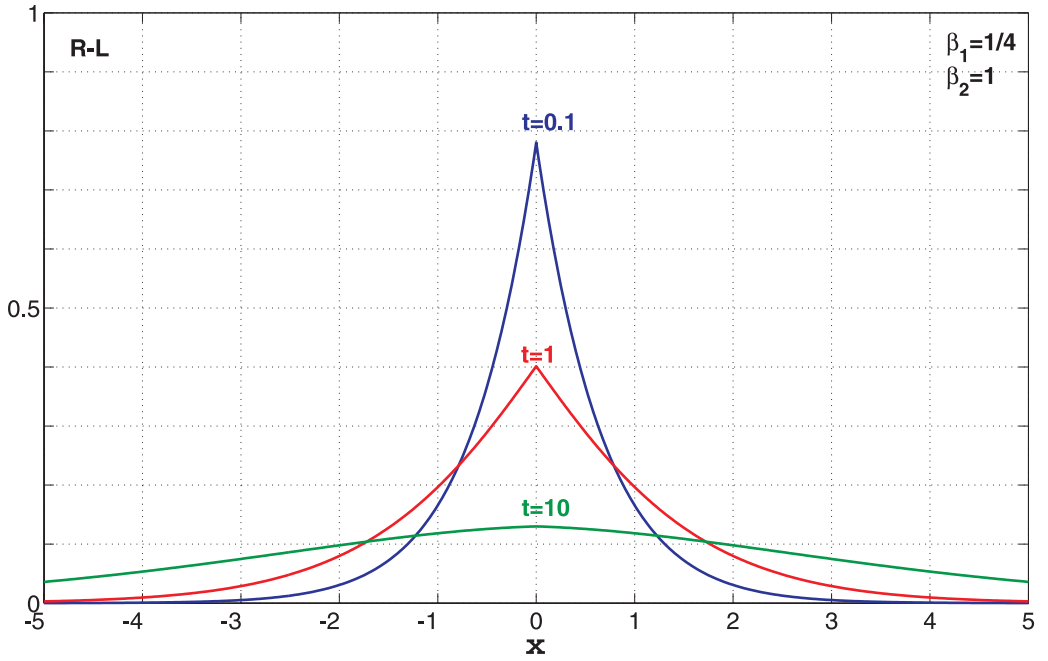


Figure 3. The fundamental solution plotted against x (in the interval $|x| \leq 5$), for the double-order distribution $\{\beta_1 = 1/4, \beta_2 = 1\}$ at times $t = 0.1, 1, 10$. Top: R-L form. Bottom: C form.

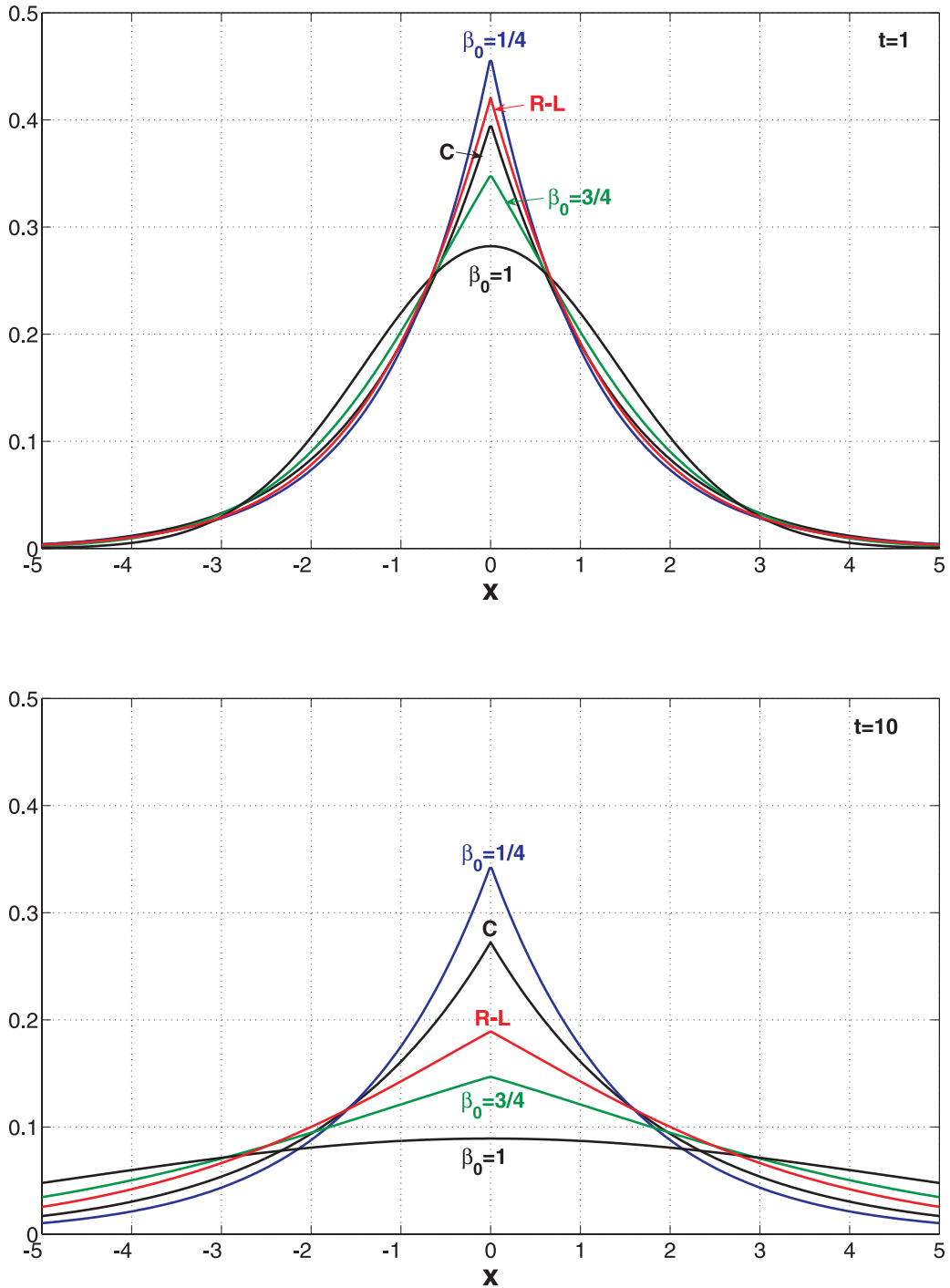


Figure 4. The fundamental solutions plotted against x (in the interval $|x| \leq 5$), for the uniform order distribution in the R-L and C forms, compared with solutions for a selection of single order cases. Top: $t = 1$. Bottom: $t = 10$.

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Dedicated to Professor Dang Dinh Ang, PhD, on occasion of his eightieth birthday.

APPENDIX A: RIEMANN-LIOUVILLE AND CAPUTO FRACTIONAL DERIVATIVES

The purpose of this Appendix is to clarify for the interested reader the main differences between the Riemann-Liouville (R-L) and Caputo (C) fractional derivatives for well-behaved functions $f(t)$ with $t \geq 0$, exhibiting a finite limit $f(0^+)$ as $t \rightarrow 0^+$

Using $\mu \in (0, 1]$ to denote the order, the R-L derivative is defined as

$${}_t D^\mu f(t) := \begin{cases} \frac{1}{\Gamma(1-\mu)} \frac{d}{dt} \int_0^t \frac{f(\tau)}{(t-\tau)^\mu} d\tau, & 0 < \mu < 1, \\ \frac{df(t)}{dt}, & \mu = 1 \end{cases} \tag{56}$$

and the C derivative as

$${}_t D_*^\mu f(t) := \begin{cases} \frac{1}{\Gamma(1-\mu)} \int_0^t \frac{f'(\tau)}{(t-\tau)^\mu} d\tau, & 0 < \mu < 1, \\ \frac{df(t)}{dt}, & \mu = 1. \end{cases} \tag{57}$$

The two fractional derivatives are related to the Riemann-Liouville fractional integral as follows. The Riemann-Liouville fractional integral is

$${}_t J^\mu f(t) := \frac{1}{\Gamma(\mu)} \int_0^t f(\tau)(t-\tau)^{\mu-1} d\tau, \quad \mu > 0 \tag{58}$$

(with the convention ${}_t J^0 f(t) = f(t)$) and is known to satisfy the semigroup property ${}_t J^\mu {}_t J^\nu = {}_t J^{\mu+\nu}$, with $\mu, \nu > 0$ For any $\mu > 0$ the Riemann-Liouville fractional derivative is defined as the left inverse of the corresponding fractional integral (like the derivative of any integer order), namely ${}_t D^\mu {}_t J^\mu f(t) = f(t)$ Thus, for $\mu \in (0, 1]$, we have

$${}_t D^\mu f(t) := {}_t D^1 {}_t J^{1-\mu} f(t), \quad {}_t D_*^\mu f(t) := {}_t J^{1-\mu} {}_t D^1 f(t) \tag{59}$$

and

$${}_t J^\mu {}_t D_*^\mu f(t) = {}_t J^\mu {}_t J^{1-\mu} {}_t D^1 f(t) = {}_t J^1 {}_t D^1 f(t) = f(t) - f(0^+). \tag{60}$$

Recalling the rule

$${}_t D^\mu t^\gamma = \frac{\Gamma(\gamma + 1)}{\Gamma(\gamma + 1 - \mu)} t^{\gamma-\mu}, \quad \mu \geq 0, \quad \gamma > -1 \tag{61}$$

it turns out that, for $0 < \mu < 1$,

$${}_t D_*^\mu f(t) = {}_t D^\mu [f(t) - f(0^+)] = {}_t D^\mu f(t) - f(0^+) \frac{t^{-\mu}}{\Gamma(1 - \mu)}. \tag{62}$$

Note that for $\mu = 1$, the two types of fractional derivative are equivalent, the constant $f(0^+)$ playing no role.

By removing the singularity in the time origin, the Caputo fractional derivative represents a sort of regularization of the Riemann-Liouville fractional derivative, and satisfies the relevant property of being zero when applied to a constant.

Let us now consider the behaviour of the above non-integer order derivatives with respect to the Laplace transformation of a function $f(t)$, which is defined as

$$\tilde{f}(s) = \mathcal{L}\{f(t); s\} := \int_0^\infty e^{-st} f(t) dt, \quad s \in \mathbb{C}. \tag{63}$$

Under suitable conditions, the Laplace transform of the first derivative of $f(t)$ is given by

$$\mathcal{L}\{{}_t D^1 f(t); s\} = s \tilde{f}(s) - f(0^+) \quad f(0^+) := \lim_{t \rightarrow 0^+} f(t). \tag{64}$$

For the Riemann-Liouville derivative of non-integer order μ , we have

$$\mathcal{L}\{{}_t D^\mu f(t); s\} = s^\mu \tilde{f}(s) - g(0^+), \quad g(0^+) := \lim_{t \rightarrow 0^+} {}_t J^{1-\mu} f(t), \quad 0 < \mu < 1 \tag{65}$$

while for the Caputo derivative of non-integer order μ we have

$$\mathcal{L}\{{}_t D_*^\mu f(t); s\} = s^\mu \tilde{f}(s) - f(0^+), \quad f(0^+) := \lim_{t \rightarrow 0^+} f(t), \quad 0 < \mu < 1. \tag{66}$$

It can be seen that rule (65) is more cumbersome in usage than rule (66), as it requires initial values for an extra function $g(t)$, which is related to the given $f(t)$ by a fractional integral. However, we can see that when the limiting value $f(0^+)$ is finite, $g(0^+)$ is negligible, and thus rule (65) simplifies to

$$\mathcal{L}\{{}_t D^\mu f(t); s\} = s^\mu \tilde{f}(s), \quad 0 < \mu < 1. \tag{67}$$

For further discussion on the theory and applications of fractional calculus, the reader is referred to the standard books on the subject by Samko et al. (1993), Miller and Ross (1993), Podlubny (1999), and also to more recent works by West et al. (2003), Zaslavsky (2005), Kilbas et al. (2006), and Magin (2006).

APPENDIX B: MITTAG-LEFFLER FUNCTIONS

B.1. The Classical Mittag-Leffler Function

The Mittag-Leffler function $E_\mu(z)$ (with $\mu > 0$) is an entire transcendental function of order $1/\mu$, defined in the complex plane by the power series

$$E_\mu(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu k + 1)}, \quad z \in \mathbb{C}. \tag{68}$$

It was introduced and studied by the Swedish mathematician Mittag-Leffler at the beginning of the 20th century to provide a noteworthy example of an entire function that generalizes the exponential (to which it reduces for $\mu = 1$) (For full details of this function, see, e.g., Erdélyi et al., 1955; Djrbashian, 1966; Samko et al., 1993; Gorenflo and Mainardi, 1997; Podlubny, 1999; Mainardi and Gorenflo, 2000; Kilbas et al., 2006). In particular, we note that the function $E_\mu(-x)$ ($x \geq 0$) returns a completely monotonic function of x if $0 < \mu \leq 1$. This property is still valid if we consider the variable $x = \lambda t^\mu$, where λ is a positive constant. Thus, the function $E_\mu(-\lambda t^\mu)$ preserves the complete monotonicity of the exponential $\exp(-\lambda t)$. Indeed, for $0 < \mu < 1$ it is represented in terms of a real Laplace transform (of a real parameter r) of the non-negative function (referred to as the spectral function)

$$E_\mu(-\lambda t^\mu) = \frac{1}{\pi} \int_0^\infty e^{-rt} \frac{\lambda r^{\mu-1} \sin(\mu\pi)}{\lambda^2 + 2\lambda r^\mu \cos(\mu\pi) + r^{2\mu}} dr. \tag{69}$$

Note that as $\mu \rightarrow 1$, the spectral function tends to the generalized Dirac function $\delta(r - \lambda)$.

Mittag-Leffler function (69) starts at $t = 0$ as a stretched exponential, and decreases for $t \rightarrow \infty$ as a power with exponent $-\mu$:

$$E_\mu(-\lambda t^\mu) \sim \begin{cases} 1 - \lambda \frac{t^\mu}{\Gamma(1+\mu)} \sim \exp\left\{-\frac{\lambda t^\mu}{\Gamma(1+\mu)}\right\}, & t \rightarrow 0^+ \\ \frac{t^{-\mu}}{\lambda \Gamma(1-\mu)}, & t \rightarrow \infty. \end{cases} \tag{70}$$

Equations (69) and (70) can also be derived from the Laplace transform pair

$$\mathcal{L}\{E_\mu(-\lambda t^\mu); s\} = \frac{s^{\mu-1}}{s^\mu + \lambda}. \tag{71}$$

In fact, it is sufficient to apply the Titchmarsh theorem ($s = re^{i\pi}$) to derive (69) and the Tauberian theory ($s \rightarrow \infty$ and $s \rightarrow 0$) to derive (70).

If $\mu = 1/2$, we have (for $t \geq 0$)

$$E_{1/2}(-\lambda\sqrt{t}) = e^{\lambda^2 t} \operatorname{erfc}(\lambda\sqrt{t}) \sim 1/(\lambda\sqrt{\pi t}), \quad t \rightarrow \infty \tag{72}$$

where erfc denotes the complementary error function (see, e.g., Abramowitz and Stegun, 1965).

B.2. The Generalized Mittag-Leffler Function

The Mittag-Leffler function in two parameters $E_{\mu,\nu}(z)$ ($\Re\{\mu\} > 0, \nu \in \mathbb{C}$) is defined by the power series

$$E_{\mu,\nu}(z) := \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\mu k + \nu)}, \quad z \in \mathbb{C}. \tag{73}$$

It generalizes the classical Mittag-Leffler function, to which it reduces for $\nu = 1$, and is an entire transcendental function of order $1/\Re\{\mu\}$.

The function $E_{\mu,\nu}(-x)$ ($x \geq 0$) is completely monotonic if $0 < \mu \leq 1$ and $\nu \geq \mu$. Again, this property is still valid if we consider the variable $x = \lambda t^\mu$ where λ is a positive constant. In this case, the asymptotic representations as $t \rightarrow 0^+$ and $t \rightarrow +\infty$ become

$$E_{\mu,\nu}(-\lambda t^\mu) \sim \begin{cases} \frac{1}{\Gamma(\nu)} - \lambda \frac{t^\mu}{\Gamma(\nu+\mu)}, & t \rightarrow 0^+ \\ \frac{1}{\lambda} \frac{t^{-\mu+\nu-1}}{\Gamma(\nu-\mu)}, & t \rightarrow \infty. \end{cases} \tag{74}$$

For $0 < \mu = \nu \leq 1$ the Laplace transform pair

$$\mathcal{L}\{t^{\nu-1} E_{\mu,\nu}(-\lambda t^\mu); s\} = \frac{s^{\mu-\nu}}{s^\mu + \lambda} \tag{75}$$

with $\mu, \nu \in \mathfrak{R}^+$, can be used (Podlubny, 1999) to derive the noteworthy identity

$$t^{-(1-\mu)} E_{\mu,\mu}(-\lambda t^\mu) = -\frac{1}{\lambda} \frac{d}{dt} E_\mu(-\lambda t^\mu), \quad 0 < \mu \leq 1. \tag{76}$$

APPENDIX C: THE EXPONENTIAL INTEGRAL AND RELATED FUNCTIONS

The exponential integral function, denoted here by $\mathcal{E}_1(z)$ (to avoid confusion with the Mittag-Leffler functions), is defined as

$$\mathcal{E}_1(z) = \int_z^\infty \frac{e^{-t}}{t} dt = \int_1^\infty \frac{e^{-zt}}{t} dt. \tag{77}$$

This function exhibits a branch cut along the negative real semi-axis, and admits the representation

$$\mathcal{E}_1(z) = -\gamma - \log z - \sum_{n=1}^{\infty} \frac{z^n}{nn!}, \quad |\arg z| < \pi \tag{78}$$

where $\gamma = 0.57721\dots$ is the Euler-Mascheroni constant. The power series on the right-hand side is absolutely convergent in all of \mathbb{C} and represents the entire function called the modified exponential integral

$$\text{Ein}(z) := \int_0^z \frac{1 - e^{-\zeta}}{\zeta} d\zeta = - \sum_{n=1}^{\infty} \frac{z^n}{n n!}. \tag{79}$$

Thus, in view of (C.2) and (C.3), we write

$$\mathcal{E}_1(z) = -\gamma - \log z + \text{Ein}(z), \quad |\arg z| < \pi. \tag{80}$$

This relation is important in understanding the analytic properties of the classical exponential integral function, in that it isolates the multi-valued part represented by the logarithmic function from the regular part represented by the entire function $\text{Ein}(z)$. In \mathfrak{R}^+ , the function $\text{Ein}(x)$ turns out to be a Bernstein function, which means that is positive and increasing, with its first derivative being completely monotonic.

The asymptotic behaviour as $z \rightarrow \infty$ of the exponential integrals can be obtained from the integral representation (77), taking note that

$$\mathcal{E}_1(z) := \int_z^{\infty} \frac{e^{-t}}{t} dt = e^{-z} \int_0^{\infty} \frac{e^{-u}}{u + z} du. \tag{81}$$

In fact, by repeated partial integrations on the right-hand side, we get

$$\mathcal{E}_1(z) \sim \frac{e^{-z}}{z} \sum_{n=0}^{\infty} (-1)^n \frac{n!}{z^n}, \quad z \rightarrow \infty \tag{82}$$

for $|\arg z| \leq \pi - \delta$. Next, we report a number of relevant Laplace transform pairs in which logarithmic and exponential integral functions are involved.

Taking $t > 0$, the basic Laplace transforms pairs are

$$\mathcal{L}\{\log t; s\} = -\frac{\gamma + \log s}{s}, \quad \Re s > 0 \tag{83}$$

$$\mathcal{L}\{\mathcal{E}_1(t); s\} = \frac{\log(s + 1)}{s}, \quad \Re s > -1. \tag{84}$$

Proof of these can be found elsewhere (see, e.g., Ghizzetti and Ossicini, 1971, pp. 104–105). We then easily derive, for $\Re s > 0$,

$$\mathcal{L}\{\gamma + \log t; s\} = -\frac{\log s}{s} \tag{85}$$

$$\mathcal{L}\{\gamma + \log t + \mathcal{E}_1(t); s\} = \frac{\log(s + 1)}{s} - \frac{\log s}{s} = \frac{\log(1/s + 1)}{s} \tag{86}$$

$$\mathcal{L}\{\gamma + \log t + e^t \mathcal{E}_1(t); s\} = \frac{\log s}{s-1} - \frac{\log s}{s} = \frac{\log s}{s(s-1)}. \quad (87)$$

We will now outline the different asymptotic behaviour of the three functions $\mathcal{E}_1(t)$, $\text{Ein}(t)$ and $\gamma + \log t + e^t \mathcal{E}_1(t)$, for small argument ($t \rightarrow 0^+$) and large argument ($t \rightarrow +\infty$). Using equations (78), (80) and (82), we have

$$\mathcal{E}_1(t) \sim \begin{cases} \log(1/t), & t \rightarrow 0^+ \\ e^{-t}/t, & t \rightarrow +\infty \end{cases} \quad (88)$$

$$\text{Ein}(t) \sim \begin{cases} t, & t \rightarrow 0^+ \\ \log t, & t \rightarrow +\infty \end{cases} \quad (89)$$

$$\gamma + \log t + e^t \mathcal{E}_1(t) \sim \begin{cases} t \log(1/t), & t \rightarrow 0^+ \\ \log t, & t \rightarrow +\infty. \end{cases} \quad (90)$$

Note that all the above asymptotic representations can be obtained from the Laplace transforms of the corresponding functions by invoking the Tauberian theory for regularly varying functions (power functions multiplied by slowly varying functions) (Feller, 1971). A (measurable) positive function $a(y)$, defined in a right neighbourhood of zero, is said to be *slowly varying at zero* if $a(y) > 0$ and $a(cy)/a(y) \rightarrow 1$ with $y \rightarrow 0$ for every $c > 0$. Similarly, a (measurable) positive function $b(y)$, defined in the neighbourhood of infinity, is said to be *slowly varying at infinity* if $b(cy)/b(y) \rightarrow 1$ with $y \rightarrow \infty$ for every $c > 0$. Consider, for example, $(\log y)^\gamma$ with $\gamma \in \mathfrak{R}$ and $\exp(\log y / \log \log y)$.

Finally, consider the Laplace transform pair

$$\mathcal{L}\{v(t, a); s\} = \frac{1}{s^{a+1} \log s}, \quad \Re s > 0 \quad (91)$$

where

$$v(t, a) := \int_0^\infty \frac{t^{a+\tau}}{\Gamma(a+\tau+1)} d\tau, \quad a > -1. \quad (92)$$

For details of this transcendental function the reader is referred to the third volume of the Handbook of the Bateman Project (Erdélyi et al., 1955, Chapter 18).

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