Monografías Matemáticas *García de Galdeano* **41**, 187–197 (2018)

Fractional Calculus as a modeling framework

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Abstract. Fractional Calculus represents a natural instrument to model nonlocal phenomena either in space or in time. From Physics and Chemistry to Biology, a vast amount processes involve different space/time scales. For many of those, the dynamics can be formulated by fractional differential equations that include the nonlocal effects. We give a panoramic view of the problem and the associated numerical challenges.

Keywords: Fractional Calculus, fractional differential equations, nonlocal effects.

AMS classification: AMS 34A08, 35R11.

§1. Introduction: fractional derivatives

The tools of Fractional Calculus are as old as calculus itself. Fractional Calculus deals with the study of so-called fractional order integral and derivative operators over real or complex domains, and their applications. Such operators emerge with the objective to generalize the concepts of integral and derivative to non-integer orders. Thus, the designation of "Integration and Derivation of Arbitrary Order" is more appropriate.

The origin of Fractional Calculus is in 1675, when Leibniz introduces the notion of n-order derivative of a function. Next, in 1695, the first published results were cited in a letter from L'Hôpital to Leibniz, where L'Hôpital exposes the question of the possible meaning of the derivative of order $n = 1/2$. The intuitive answer of Leibniz was: "It would seem that very useful consequences will be extracted some day from these paradoxes, since there is no paradox without usefulness."[1]

From this moment on, many mathematicians have studied this topic and they have given their contributions to the development of the Fractional Calculus. Among others, we can cite Euler, Lagrange, Fourier, Abel, Liouville, Riemann, Grünwald, Letnikov, Holmgren, Cauchy, Hadamard, Hardy, Riesz, Weyl...

A first approximation to the concept of fractional derivative can be taken from the classical definition of derivative of different orders:

$$f'(x) = \lim_{h\to 0} \frac{f(x+h) - f(x)}{h} \tag{1}$$

$$\begin{aligned} f''(x) &= \lim_{h\to 0} \frac{f'(x+h) - f'(x)}{h} \\ &= \lim_{h_1\to 0} \frac{\lim_{h_2\to 0} \frac{f(x+h_1+h_2)-f(x+h_1)}{h_2} - \lim_{h_2\to 0} \frac{f(x+h_2)-f(x)}{h_2}}{h_1} \\ &= \lim_{h\to 0} \frac{f(x+2h) - 2f(x+h) + f(x)}{h^2} \end{aligned} \tag{2}$$

$$\frac{d^n f}{dx^n}(x) = \lim_{h\to 0} \frac{\sum_{0\le m\le n}(-1)^m\binom{n}{m} f(x+(n-m)h)}{h^n}, \quad \text{where } \binom{n}{k} = \frac{n!}{k!(n-k)!}, \quad 0 \le k \le n \tag{3}$$

If we consider the generalization of the concept of factorial through the function Gamma, which we will analyze in the following section, we obtain the definition of fractional derivative of Grünwald-Letnikov:

$$D^q f(x) = \lim_{h\to 0} \frac{1}{h^q} \sum_{m=0}^{\infty} (-1)^m \binom{q}{m} f(x+(q-m)h), \qquad x, h \in \mathbb{R}, q \in \mathbb{N}, \tag{4}$$

$$D^\alpha f(x) = \lim_{h\to 0} h^{-\alpha} \sum_{m=0}^{\frac{x-a}{h}} (-1)^m \frac{\Gamma(\alpha+1)}{m!\Gamma(\alpha-m+1)} f(x-mh), \qquad x \in [a,b], h > 0, \alpha \in \mathbb{R}^+. \tag{5}$$

Another important definition of the fractional integral and derivative corresponds to Riemann-Liouville:

- Left-side Riemann-Liouville Fractional Integral of order $\alpha > 0$:

$$_aD_x^{-\alpha}\phi(x) = \frac{1}{\Gamma(\alpha)} \int_a^x (x-t)^{\alpha-1}\phi(t)dt, \qquad x > a. \tag{6}$$

- Right-side Riemann-Liouville Fractional Integral of order $\alpha < 0$:

$$_xD_b^{-\alpha}\phi(x) = \frac{1}{\Gamma(\alpha)} \int_x^b (x-t)^{\alpha-1}\phi(t)dt, \qquad x < b. \tag{7}$$

- Left-side Riemann-Liouville Fractional Derivative of order $\alpha > 0$:

$$_aD_x^{\alpha}\phi(x) = \frac{1}{\Gamma(n-\alpha)} \left(\frac{\partial}{\partial x}\right)^n \int_a^x (x-t)^{\alpha-(n-1)}\phi(t)dt, \qquad x > a. \tag{8}$$

- Right-side Riemann-Liouville Fractional Derivative of order $\alpha < 0$:

$$_xD_b^{\alpha}\phi(x) = \frac{1}{\Gamma(n-\alpha)} \left(-\frac{\partial}{\partial x}\right)^n \int_x^b (x-t)^{\alpha-(n-1)}\phi(t)dt, \qquad x < b. \tag{9}$$

In all cases $n \in \mathbb{N}$, such that $0 \le n - 1 < \alpha < n$.

Related to the integrals of Riemann-Liouville, the definition of Caputo fractional derivative appears:

- Left-side Caputo Fractional Derivative of order $\alpha > 0$:

$$
\begin{aligned}
{}_{a}^{C}D_{x}^{\alpha}\phi(x) &= {}_{a}D_{x}^{\alpha}\left(\phi(x) - \sum_{k=0}^{n-1} \frac{\phi^{(k)}(a)}{k!}(x-a)^{k}\right) \\
&= \frac{1}{\Gamma(n-\alpha)} \int_{a}^{x} \frac{\phi^{(n)}(t)}{(x-t)^{\alpha+1-n}} dt, \qquad x > a.
\end{aligned} \tag{10}
$$

- Right-side Caputo Fractional Derivative of order $\alpha < 0$:

$$
{}_{x}^{C}D_{b}^{\alpha}\phi(x) = \frac{(-1)^{n}}{\Gamma(n-\alpha)} \int_{x}^{b} \frac{\phi^{(n)}(t)}{(x-t)^{\alpha+1-n}} dt, \qquad x < b. \tag{11}
$$

We have, as before, $n \in \mathbb{N}$ such that $0 \le n - 1 < \alpha < n$, and now the $n + 1$ derivatives of function ϕ must be continuous and bounded in $[a, b]$.

A basic consideration related to these operators is that they allow to introduce memory terms in a natural form. This can be shown through Calculus Fundamental Theorem:

$$
\frac{dx}{dt} = F(t), \qquad x(0) = x_0, \tag{12}
$$

can be expressed in integral form as

$$
x(t) = x_0 + \int_{0}^{t} 1 \cdot F(\tau) d\tau. \tag{13}
$$

Substituting constant 1 by a convolution kernel introduces the memory term:

$$
x(t) = x_0 + \int_{0}^{t} K(t-\tau) \cdot F(\tau) d\tau \tag{14}
$$

and we can consider this as a base to construct other possible definitions for fractional integrals.

1.1. From Factorial to the Gamma Function

The Gamma function is a function that generalizes the definition of the factorial to non-positive numbers. Its definition is:

$$
\Gamma(z) = \int_{0}^{\infty} s^{z-1} e^{-s} ds \tag{15}
$$

for any complex number z with positive real part.

Using integration by parts in (15), a fundamental property of the Gamma function is obtained:

$$
\Gamma(z) = (z-1)\Gamma(z-1), \tag{16}
$$

which allows to give the Gamma function of a positive integer number as

$$\Gamma(n) = (n-1)!\,. \tag{17}$$

In this context, the Gamma function is a generalization of the concept of factorial.

Now, if we introduce this in the derivative of a monomial function and we study both the ordinary and fractional case with the fractional derivative of Riemann-Liouville, we observe that the fractional generalization can be made formally as:

$$\frac{d^n}{dx^n}x^m = \frac{m!}{(m-n)!}x^{m-n} \quad \Rightarrow \quad \frac{d^\alpha}{dx^\alpha}x^\mu = \frac{\Gamma(\mu+1)}{\Gamma(\mu-\alpha+1)}x^{\mu-\alpha}. \tag{18}$$

Special functions related to the eigenfunctions of fractional operators are the Mittag-Leffler functions. They appear in the solution of many fractional differential equations. The Mittag-Leffler functions are generalizations of the exponential function and they was introduced by the mathematician G.M. Mittag-Leffler in 1903:

$$\begin{aligned} E_\alpha(t) &= \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(\alpha k+1)} \qquad (\alpha > 0, \alpha \in \mathbb{R}), \\ E_{\alpha,\beta}(t) &= \sum_{k=0}^{\infty} \frac{t^k}{\Gamma(\alpha k+\beta)} \qquad (\alpha,\beta > 0, \alpha,\beta \in \mathbb{R}). \end{aligned} \tag{19}$$

For some values of the parameters α,β, Mittag-Leffer functions return known classical functions, for example:

$$E_1(t) = e^t, \tag{20}$$

$$E_2(t) = \cosh(\sqrt{t}). \tag{21}$$

The relevance of the Mittag-Lefler functions is their behavior as generalized exponential functions associated to the Riemann-Liouville and Caputo fractional derivatives:

$${}_0D_t^\alpha t^{\alpha-1}E_{\alpha,\alpha}(\lambda t^\alpha) = \lambda t^{\alpha-1}E_{\alpha,\alpha}(\lambda t^\alpha), \tag{22}$$

and

$${}_0^CD_t^\alpha E_\alpha(\lambda t^\alpha) = \lambda E_\alpha(\lambda t^\alpha). \tag{23}$$

§2. New mathematical scenarios: new families of functions and equations.

Fractional Calculus presents many applications in different areas, as it is shown in the book [2]:

"The purpose of this book is to explore the behavior of biological systems from the perspective of fractional calculus. Fractional calculus, integration and differentiation of an arbitrary or fractional order, provides new tools that expand the descriptive power of calculus beyond the familiar integer-order concepts of rates of change and area under a curve."

"Fractional Calculus adds new functional relationships and new functions to the familiar family of exponentials and sinusoids that arise in the realm of ordinary linear differential equations."

Fractals and Fractional Calculus generate parameters of intermediate order: dimensions for the former, arbitrary integration and differentiation orders for the latter. This has been deeply studied in the literature ([3], [7]), allowing to achieve a better modeling for many different applications.

For instance, let us consider the following contexts in the Classical Physics, whose basic equations are the following:

- Hooke Law: $F(t) = kx(t)$
- Newtonian Fluid: $F(t) = k\frac{dx}{dt}(t)$
- Newton second law: $F(t) = k\frac{d^2x}{dt^2}(t)$

As an interpolation of these equations, a fractional approach gives the possibility to look for intermediate or mixed behaviours:

$$F(t) = k\frac{d^\alpha x}{dt^\alpha}(t) \tag{24}$$

Some other contexts are the diffusion processes associated to the basic diffusion equation:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \tag{25}$$

as we show in the following table:

Law	Darcy: $\vec{q} = -K\ \overrightarrow{\text{Grad}}\ h$	Fourier: $\vec{Q} = -\kappa\ \overrightarrow{\text{Grad}}\ T$	Fick: $\vec{f} = -D\ \overrightarrow{\text{Grad}}\ C$	Ohm: $\vec{j} = -\sigma\ \overrightarrow{\text{Grad}}\ V$
Flux	Subterranean Water: q	Heat: Q	Solute: f	Charge: j
Potential	Hydrostatic Charge: h	Temperature: T	Concentration: C	Voltage: V
Medium's Property	Hydraulic Conductivity: K	Thermal Conductivity: κ	Diffusion Coefficient: D	Electric Conductivity: σ

The diffusion equation can be generalized through the fractional operators that allow to make a natural interpolation among equations, starting with the first order wave equation and ending with the second order wave equation:

$$\text{First order wave equation (hyperbolic): } \frac{\partial u}{\partial t} = \frac{\partial u}{\partial x} \tag{26}$$

$$\text{Interpolation: } \frac{\partial u}{\partial t} = \frac{\partial^\alpha u}{\partial x^\alpha} \tag{27}$$

$$\text{Diffusion equation (parabolic): } \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} \tag{28}$$

$$\text{Interpolation: } \frac{\partial^\alpha u}{\partial t^\alpha} = \frac{\partial^2 u}{\partial x^2} \tag{29}$$

$$\text{Wave Equation (hyperbolic): } \frac{\partial^2 u}{\partial t^2} = \frac{\partial^2 u}{\partial x^2} \tag{30}$$

Another fractional approach associated to the previous one is the use of Dirac-type fractional equations according to the following scheme:

$$\begin{tikzcd}
A\dfrac{\partial \psi}{\partial t} + B\dfrac{\partial \psi}{\partial x} = 0 \arrow[rr, "A\frac{\partial^\alpha \psi}{\partial t^\alpha} + B\frac{\partial \psi}{\partial x} = 0", "\psi = \begin{pmatrix} \varphi \\ \xi \end{pmatrix}"'] & & A\dfrac{\partial^{1/2} \psi}{\partial t^{1/2}} + B\dfrac{\partial \psi}{\partial x} = 0 \\
\dfrac{\partial^2 u}{\partial t^2} - \dfrac{\partial^2 u}{\partial x^2} = 0 \arrow[u, "\begin{matrix} A^2 = I \\ B^2 = I \\ \{A, B\} = 0 \end{matrix}"] \arrow[rr, "\gamma = 2\alpha", "\frac{\partial^\gamma u}{\partial t^\gamma} - \frac{\partial^2 u}{\partial x^2} = 0"'] & & \dfrac{\partial u}{\partial t} - \dfrac{\partial^2 u}{\partial x^2} = 0 \arrow[u]
\end{tikzcd}$$

In this way, equation

$$A\frac{\partial^{1/2} \psi}{\partial t^{1/2}} + B\frac{\partial \psi}{\partial x} = 0 \tag{31}$$

can be interpreted as the description of two coupled diffusion processes or a diffusion process with internal degrees of freedom. In this equation, each component, φ and ξ, satisfies the standard diffusion equation and they are named *diffunors* similarly to the *spinors* of the Quantum Mechanic. This provides another form of studying the interpolation between the hyperbolic operator of the wave equation and the parabolic one of the classical diffusion equation. Depending on the chosen representation of the Pauli Algebra, that A and B must verify, we obtain a system of equations coupled or decoupled:

$$A_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad B_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \Longrightarrow \quad \begin{cases} \partial_t^\alpha \varphi = \varphi \\ \partial_t^\alpha \xi = -\xi \end{cases} \tag{32}$$

$$A_2 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad B_2 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \quad \Longrightarrow \quad \begin{cases} \partial_t^\alpha \varphi = \xi \\ \partial_t^\alpha \xi = \varphi \end{cases} \tag{33}$$

$$A\frac{\partial^\alpha \psi}{\partial t^\alpha} + B\frac{\partial \psi}{\partial x} = 0 \xrightarrow{\gamma = 2\alpha} \frac{\partial^\gamma u}{\partial t^\gamma} - \frac{\partial^2 u}{\partial x^2} = 0$$

In the study of the temporal inversion ($t \to -t$), we have:

- If $\alpha = 1$, we have that both the Dirac and wave equations are invariant by temporal inversion.
- If $\alpha = 1/2$, the classical diffusion equation and its square root are not invariant by temporal inversion.

- Interpolation in: $0 < \alpha < 1$. The invariance by temporal inversion is satisfied only for some specific values
  - Fractional Dirac Equation:
    $\alpha = \frac{1}{3}, \frac{1}{5}, \frac{1}{7}, \ldots, \frac{3}{5}, \frac{3}{7}, \frac{3}{9}, \ldots, \frac{5}{7}, \frac{5}{9}, \frac{5}{11}, \ldots$
  - Fractional Diffusion Equation:
    $\alpha = \frac{1}{3}, \frac{2}{3}, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, \frac{1}{7}, \frac{2}{7}, \ldots, \frac{6}{7}, \frac{1}{9}, \ldots$

In the study of the space-temporal inversion ($x \to -x$, $t \to -t$), both equations are invariant by spatial inversion and in the interpolation $0 < \alpha < 1$, the invariance by space-temporal inversion is satisfied for the same values of α in both equations:

$$\alpha = \frac{1}{3}, \frac{2}{3}, \frac{1}{5}, \frac{2}{5}, \frac{3}{5}, \frac{4}{5}, \frac{1}{7}, \frac{2}{7}, \ldots, \frac{6}{7}, \frac{1}{9}, \ldots$$

The fractional Dirac equation is not invariant by temporal translations due to the non-local character of the time fractional derivative.

Some other fractional differential equations are obtained by considering the root $1/3$ of both the Wave and Diffusion Equations:

$$\text{Wave Equation: } P\partial_t^{2/3}\varphi + Q\partial_x^{2/3}\varphi = 0 \tag{34}$$

$$\text{Diffusion Equation: } P\partial_t^{1/3}\varphi + Q\partial_x^{2/3}\varphi = 0 \tag{35}$$

where

$$P^3 = I \qquad Q^3 = -I \qquad PPQ + PQP + QPP = 0 \qquad QQP + QPQ + PQQ = 0 \tag{36}$$

A possible realization is in terms of the 3×3 matrices associated to the Silvester Algebra:

$$P = \begin{pmatrix} 0 & 0 & 1 \\ \omega^2 & 0 & 0 \\ 0 & \omega & 0 \end{pmatrix}, \quad Q = \Omega \begin{pmatrix} 0 & 0 & 1 \\ \omega & 0 & 0 \\ 0 & \omega^2 & 0 \end{pmatrix}, \tag{37}$$

with ω a cubic root of the unity and Ω a cubic root of the negative unity. In this case, φ has three components.

As an example of the associated mathematical problems, let us consider the Cauchy general problem in the space of the functions whose Laplace and Fourier transforms exist, $LF = L(R^+) \times F(R)$:

$$^{C}D_t^{\alpha}u(t,x) - \lambda^{L}D_x^{\beta}u(t,x) = 0, \quad t > 0, x \in \mathbb{R}, 0 < \alpha \leq 1, \beta > 0, \tag{38}$$

$$\lim_{x \to \pm\infty} u(t,x) = 0, \quad u(0+,x) = g(x), \tag{39}$$

where $^{C}D_t^{\alpha}$ is the Caputo fractional partial derivative, defined as:

$$D_t^{\alpha}u(t,x) = {}^{C}D_t^{\alpha}u(t,x) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u_\tau(\tau,x)}{(t-\tau)^{\alpha}} d\tau \tag{40}$$

and where D_x^{β} is the Riemann-Liouville fractional partial derivative:

$$D_x^{\beta}u(t,x) = {}^{L}D_x^{\beta}u(t,x) = \frac{1}{\Gamma(m-\beta)} \frac{\partial^m}{\partial x^m} \int_{-\infty}^{x} \frac{u(t,z)}{(x-z)^{\beta-m+1}} dz \tag{41}$$

with $m \in \mathbb{N}$, $0 \leq m-1 < \beta \leq m$.

The solution to the Cauchy problem is given by:

$$u(t,x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} G(k) E_\alpha(\lambda(-ik)^\beta t^\alpha) e^{-ikx} dk \tag{42}$$

where $G(k)$ is the Fourier transform of $g(x)$ and E_α is the Mittag-Leffler function (19). As an example, for $\beta = 1$ and $g(x) = e^{-\mu|x|}$, $\mu > 0$, the solution is:

$$u(t,x) = e^{-\mu|x|} E_\alpha(-\mu\lambda t^\alpha). \tag{43}$$

The momenta of the fundamental solution ($g(x) = \delta(x)$, $G(k) = 1$) for the case $\beta = 1$ are obtained as

$$< x^n >= \int_{-\infty}^{\infty} x^n u(t,x) dx = (-\lambda t^\alpha)^n \frac{\Gamma(n+1)}{\Gamma(\alpha n + 1)}, \qquad n = 0, 1, 2, \ldots \tag{44}$$

§3. Nonlocal phenomena in space and/or time. Applications.

3.1. Non locality

We use the term non-locality if what happens in a spatial point or at a given time depends on an average over an interval that contains that value. Thus, the non-local effects in space correspond to long-range interactions (many spatial scales), while the non-local effects in time suppose memory or delay effects (many temporal scales).

These phenomena are associated to integral or integro-differential equations, which appear in multiple contexts:

- Potential theory: Newton and Coulomb laws of the inverse of the square of the distance.
- Problems in Geophysics: three-dimensional maps of the Earth's inside.
- Problems in Electricity and Magnetism.
- Hereditary Phenomena in Physics (materials with memory: hysteresis) and Biology (ecological processes: accumulation of metals).
- Problems of Evolution of Populations.
- Problems of Radiation.
- Optimization, Control Systems.
- Communication Theory.
- Mathematical Economy.

These different phenomena can be described by fractional differential equations, and it sets out two fundamental questions:

1. *Are the models with space and/or time fractional derivatives consistent with the fundamental laws and symmetries of Nature?*
2. *How can the fractional differentiation order be experimentally observed and how does a fractional derivative emerge from models without fractional derivatives?*

For instance, we saw above that some fractional equations arise as interpolation between basic equations of Classical Physics. It is interesting to remark that, for instance, interpolation equation (29) verifies the second law of thermodynamics only if the following condition is satisfied [4]:

$$\frac{\partial^{\alpha-1} u}{\partial x^{\alpha-1}} \frac{\partial u}{\partial x} > 0. \tag{45}$$

3.2. Relaxation Processes

The fractional equations play an important role in the relaxation processes, as for instance the processes associated to viscoelastic materials. In these processes, the modeling in the context of classical mechanics consists in a combination of springs and dampers:

$$\text{Springs: Hooke Law } \sigma(t) = E\varepsilon(t) \tag{46}$$

$$\text{Dampers: Newtonian Fluid Law } \sigma(t) = \eta \frac{d\varepsilon(t)}{dt} \tag{47}$$

where

$$\sigma = \text{Tension;} \tag{48}$$

$$\epsilon = \text{Deformation;} \tag{49}$$

$$E = \text{Elastic constant or Young Modulo;} \tag{50}$$

$$\nu = \text{Viscosity Coefficient;} \tag{51}$$

so that the constitutive equation is given by the Maxwell model

$$\frac{d\varepsilon}{dt} = \frac{\sigma}{\eta} + \frac{1}{E}\frac{d\sigma}{dt}. \tag{52}$$

The relaxation module, defined as $\phi(t) = Ee^{-tE/\eta}$, indicates how the tension by unity of applied deformation varies.

Between the elastic and viscous limits we may introduce a general fractional interpolation:

$$\sigma(t) = E\tau^{\beta} \frac{d^{\beta}\varepsilon(t)}{dt^{\beta}}. \tag{53}$$

The Process of Standard Relaxation (Maxwell-Debye) is formulated through an initial value problem

$$\tau \frac{d\phi(t)}{dt} = -\phi(t), \qquad t > 0, \quad \phi(0) = \phi_0, \tag{54}$$

whose solution is

$$\phi(t) = \phi_0 e^{-t/\tau}. \tag{55}$$

Another initial formulation for the fractional generalization is

$$\phi(t) - \phi_0 = -\tau^{-1} \int_0^t \phi(t')dt' = -\tau^{-1} \frac{d^{-1}\phi(t)}{dt^{-1}}. \tag{56}$$

Formally:

$$\phi(t) - \phi_0 = -\tau^{-\beta} {}_0D_t^{-\beta} \phi(t) \tag{57}$$

where ${}_0D_t^{-\beta}$ is the Riemann-Liouville operator.

There are also deviations of the Classical Process of Maxwell-Debye Relaxation that are formulated through an initial value problem:

- Kohlrausch-Williams-Watts (KWW) decay

$$\phi(t) = \phi_0 e^{-(t/\tau)^\alpha}, \qquad 0 < \alpha < 1. \tag{58}$$

- Nutting potential law:

$$\phi(t) = \frac{\phi_0}{(1 + \frac{t}{\tau})^n}, \qquad 0 < n < 1. \tag{59}$$

These models are used in relaxation processes of deformation in materials and many transition experiments have been developed between the two behaviors.

Another context of possible application of the fractional models is the propagation of solar radiation in a planetary atmosphere [5, 6, 8, 9].

Acknowledgements

The authors thank to the support of MINECO of Spain, through the grant ESP2016-79135-R.

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