

Diffusion problems on fractional nonlocal media

Research Article

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Received 30 January 2013; accepted 30 October 2013

Abstract: In this paper, the nonlocal diffusion in one-dimensional continua is investigated by means of a fractional calculus approach. The problem is set on finite spatial domains and it is faced numerically by means of fractional finite differences, both for what concerns the transient and the steady-state regimes. Nonlinear deviations from classical solutions are observed. Furthermore, it is shown that fractional operators possess a clear physical-mechanical meaning, representing conductors, whose conductance decays as a power-law of the distance, connecting non-adjacent points of the body.

PACS (2008): 44.10.+i; 11.10.Lm

Keywords: nonlocal media • fractional calculus • heat conduction
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1. Introduction

Nonlocal theories were introduced to remove some inconsistencies related to classical mechanics, characterized by the absence of a material length scale [1]. The term "nonlocal" denotes the presence of interactions, which decay with the distance, between non-adjacent points of the body. Different approaches, considering different attenuation functions (see for instance [2] and related references), have been developed since the pioneering paper by Eringen [1]. Only recently, by implementing a power-law decaying relationship, a few models based on fractional calculus have been proposed. They are applied both to statics [3, 4], studying the stress field of a nonlocal bar under tensile load, and to dynamics [5–10], investigating anomalous wave propagation. Accord-

ing to these works, mainly related to the unidimensional case, fractional space derivatives replace the standard ones or represent an adding term in the governing equations. A clear mechanical meaning was detected in [11]: the fractional operators represent springs, with distance-decreasing stiffness, connecting non-adjoining points of the body.

On the other hand, in the context of nonlocality, lower attention has been paid so far to diffusion problems. Indeed, the problem has been generally faced analytically, investigating the existence and uniqueness of solutions as different boundary conditions are imposed [12]. From a physical point of view, anomalous diffusion is generally related to non-Markovian characteristics of the systems such as fractality, interactions and memory effects [13]. As concerns fractional calculus modelling, it is worth observing that since the operators have a simple definition in terms of their Laplace and Fourier transforms, the problem is generally set on infinite domains [14–16]. Moreover, most fractional calculus applications to diffusion models involve the fractional time derivative, where the presence

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of non-integer operators is assumed *a priori* [17–20] to model memory effects. Regarding more recent applications, it is important to mention the innovative studies in magnetic resonance [21]: a fractional generalization of Bloch equation has been proposed to understand more deeply the effects of anomalous diffusion and relaxation observed in nuclear magnetic resonance studies of materials structured over more than one length scale. The model was later modified to take into account also time delays [22, 23]. Noteworthy are also the studies on influence of the ions on the electrochemical impedance of a cell: a fractional drift-diffusion problem was solved to account for the large variety of the diffusive regimes in a real cell [24, 25].

In the present paper, the diffusion equation in fractional nonlocal media is consistently derived. For the sake of simplicity, the analysis will refer to the heat conduction process. By properly choosing the attenuation function in the nonlocal Fourier's law, through the conservation law for the internal energy, the governing diffusion equation is obtained. Suitable boundary condition are imposed. Setting the problem on a finite spatial domain, different cases are investigated numerically both in the transient and in the steady-state regimes. The solutions, for different fractional orders α , are compared to the classical ones, recovered by imposing the condition $\alpha = 2$. The physical interpretation of fractional operators concludes the work, extending the original results raising from the static analysis [11].

2. Nonlocal fractional diffusion models

According to nonlocal diffusion models, the flux $q(x)$ at a given point depends on the temperature $T(x)$ in a neighbourhood of that point by means of a convolution integral. This dependence is described by a proper attenuation function g , which decays along with the distance. In the case of a one-dimensional domain (i.e. a bar), nonlocal Fourier's law reads:

$$q(x) = -k c_\alpha \int_a^b \nabla T(y) g(x-y) dy, \quad (1)$$

where $x = a$ and $x = b$ are the bar extreme coordinates, k is the material's thermal conductivity, c_α is a material constant and ∇ is the gradient operator with respect to the spatial variable. The bar length is $L = b - a$.

By assuming the attenuation function g equal to [11]

$$g(\xi) = \frac{1}{2\Gamma(2-\alpha)|\xi|^{\alpha-1}}, \quad (2)$$

with $1 < \alpha < 2$, relation (1) becomes

$$q(x) = -k c_\alpha I_{a,b}^{2-\alpha} (\nabla T). \quad (3)$$

The operator $I_{a,b}^\beta$ represents the fractional Riesz integral ($\beta > 0$, [26]):

$$I_{a,b}^\beta f(x) = \frac{1}{2} \left[I_{a+}^\beta f(x) + I_{b-}^\beta f(x) \right] = \frac{1}{2\Gamma(\beta)} \int_a^b \frac{f(y)}{|x-y|^{1-\beta}} dy, \quad (4)$$

being I_{a+}^β and I_{b-}^β the left and right Riemann-Liouville fractional integrals (see Eqs. (1A) and (2A) in the Appendix), respectively. According to the choice (2), the internal length c_α possesses anomalous physical dimensions $[L]^{\alpha-2}$: a fractal interpretation based on the analysis performed in [27–29] may then be argued. Further studies are in progress. Notice that the following condition must hold, for the sake of completeness: $c_\alpha = 1$ for $\alpha = 2$. Thus, in this case, Eq. (3) reverts consistently to the classical Fourier's relationship $q = -k \nabla T$.

By substituting Eq. (3) into the conservation law for the internal energy:

$$\frac{\partial}{\partial t} \int_a^b \rho c T dx = -[q(x, t)]_{x=a}^{x=b} + \int_a^b S(x, t) dx, \quad (5)$$

after some analytical manipulations, we get:

$$\frac{\partial T(x, t)}{\partial t} = \frac{\bar{D} c_\alpha}{2} \{ D_{a+}^\alpha [T(x, t) - T(a, t)] \\ + D_{b-}^\alpha [T(x, t) - T(b, t)] \} + s(x, t), \quad (6)$$

where t is the time variable, $\bar{D} = k/\rho c$ is the diffusion coefficient (ρ being the bar volumetric density and c being the specific heat capacity), and D_{a+}^β and D_{b-}^β are the left and right Riemann-Liouville fractional derivatives with respect to the spatial variable x (Eqs. (5A) and (6A) in the Appendix). Eventually, the term $s = S/\rho c$ takes into account the presence of sources of energy inside the body. Equation (6) represents a fractional differential equation [30] in space. Note that, while the left fractional derivative coincides always with its integer order counterpart when the order of derivation is an integer number, the right fractional derivative coincides with the corresponding integer derivative only when the order of derivation is even; when the order of derivation is an odd number, it is equal to its opposite (see Appendix). Thus the term in the curly brackets (which, unless a constant term, coincides with the Riesz fractional derivative [26]) is equal to $2\partial^2 T / \partial x^2$ when $\alpha = 2$ (thus Eq. (6) reverts to the classical heat equation), and vanishes when $\alpha = 1$ (thus leading to a

trivial condition providing a constant temperature field in time throughout the body). Suitable initial and boundary conditions must be assigned to Eq. (6):

$$T(x, t = 0) = T_0(x), \quad (7)$$

$$\begin{aligned} T(x = a, t) &= T_a(t), \\ \text{or } q(x = a, t) &= k c_\alpha D_{a-}^{\alpha-1} [T(x, t) - T(b, t)]_{x=a} = q_a(t), \end{aligned} \quad (8)$$

$$\begin{aligned} T(x = b, t) &= T_b(t), \\ \text{or } q(x = b, t) &= -k c_\alpha D_{a+}^{\alpha-1} [T(x, t) - T(a, t)]_{x=b} = -q_b(t). \end{aligned} \quad (9)$$

In other words, the boundary conditions on the heat flux (8) and (9) are expressed by Caputo's right fractional derivative evaluated in the left extreme and by Caputo's left fractional derivative evaluated in the right extreme [27]. Of course, they are integral-type boundary conditions. By substituting Eq. (4A) into Eq. (9) (observe that $\alpha - 1 < 1$), we get, for instance:

$$\begin{aligned} q(b, t) &= \\ &\frac{k c_\alpha}{\Gamma(2-\alpha)} \left[\frac{T(b)-T(a)}{(b-a)^{2-\alpha}} + (2-\alpha) \int_a^b \frac{T(b)-T(x)}{(b-x)^{2+\alpha}} dx \right] = q_b(t). \end{aligned} \quad (10)$$

The analysis has been focused so far on the heat conduction problems, but it can easily generalized to any diffusion process. Examples include: a) infiltration of fluids on porous media, for which the scalar unknown is the fluid pressure whilst k is the permeability of the medium (Eq. (3) representing the generalization of Darcy's law); b) electrical conduction, for which the scalar is the potential, whilst k represents the electrical conductivity (Eq. (3) generalizing the classical Ohm's law).

3. Numerical implementation and results

In the following, the heat equation (6) is solved by numerical schemes. Different expressions were proposed to approximate fractional operators with order comprised between 1 and 2 [31–33]: the so-called L2 algorithm [33, 34] is here implemented. Let us introduce a partition of the interval $[a, b]$ on the x axis made of n ($n \in \mathbb{N}$) intervals of length $\Delta x = L/n$. The generic point of the partition has the abscissa x_i , with $i = 1, \dots, n+1$ and $x_1 = a$, $x_{n+1} = b$; that is, $x_i = a + (i-1)\Delta x$. Hence, for the inner points of the domain ($i = 2, \dots, n$), the discrete form of Eq.(6) reads ($1 \leq \alpha < 2$)

$$\begin{aligned} T_t(x_i, t_j) \approx \frac{\bar{D} c_\alpha}{2} \frac{(\Delta x)^{-\alpha}}{\Gamma(3-\alpha)} &\left\{ \frac{2-\alpha}{(i-1)^{\alpha-1}} (T_{2,j} - T_{1,j}) + \sum_{k=0}^{i-2} (T_{i-k+1,j} - 2T_{i-k,j} + T_{i-k-1,j}) [(k+1)^{2-\alpha} - k^{2-\alpha}] \right. \\ &\left. - \frac{2-\alpha}{(n-i+1)^{\alpha-1}} (T_{n+1,j} - T_{n,j}) + \sum_{k=0}^{n-i} (T_{i+k+1,j} - 2T_{i+k,j} + T_{i+k-1,j}) [(k+1)^{2-\alpha} - k^{2-\alpha}] \right\}, \end{aligned} \quad (11)$$

where $T_{i,j} = T(x_i, t_j)$ and $t_j = j\Delta t$, Δt representing the discrete time step.

Before proceeding, it is important to make some simple considerations about the parametric analysis. By expressing the initial condition as $T(x, 0) = T_0 f(x/L)$, being T_0 a reference temperature value, the temperature field T throughout the body results to be a function of nine parameters:

$$T = T(x, L, t, T_0, T_a, T_b, c_\alpha, \bar{D}, \alpha). \quad (12)$$

Let us define the dimensionless temperature T^* by normalizing T with respect to a suitable combination of T_0 , T_a

and T_b , depending on the specific problem under examination. A straightforward application of Buckingham theorem allows us reducing the dependency of T^* to four dimensionless parameters:

$$T^* = T^* \left(x^* = \frac{x}{L}, t^* = \frac{t \bar{D}}{L^2}, c_\alpha^* = c_\alpha L^{2-\alpha}, \alpha \right). \quad (13)$$

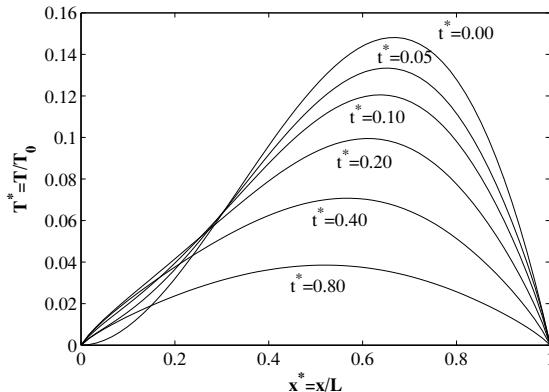


Figure 1. Dimensionless temperature field at different dimensionless time instants for a fractional bar with $\alpha = 1.5$.

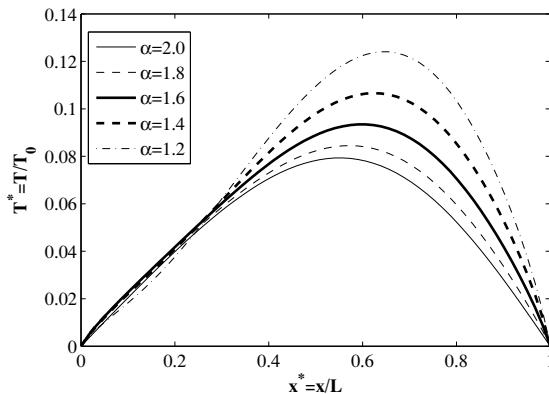


Figure 2. Dimensionless temperature field at $t^* = 0.20$ for fractional bars with different orders α .

3.1. Transient solution

Let us start by considering the transient solution related to the initial condition $f(x^*) = -(x^*)^3 + (x^*)^2$ and to homogeneous boundary conditions. It is thus reasonable to express the dimensionless temperature as $T^* = T/T_0 = f(x^*)$. The fractional parameter used for computations is: $c_\alpha^* = \pi^{2-\alpha}$. Moreover the number of intervals n is chosen equal to 60: according to the analysis performed in [33], the order of the numerical error should be less than 0.1%. The diagrams at different instants of time t^* are reported in Fig. 1 for a fractional exponent $\alpha = 1.5$. On the other hand, in Fig. 2 the curves for different α at a fixed time $t^* = 0.20$ are plotted. Notice that for α -values tending to unity, the temperature field T^* tends to $f(x^*)$, since for $\alpha = 1$ the solution is independent of time. It can thus be argued that the steady-state solution is reached before by imposing $\alpha = 2$: the lower the fractional exponent, the lower the conduction velocity.

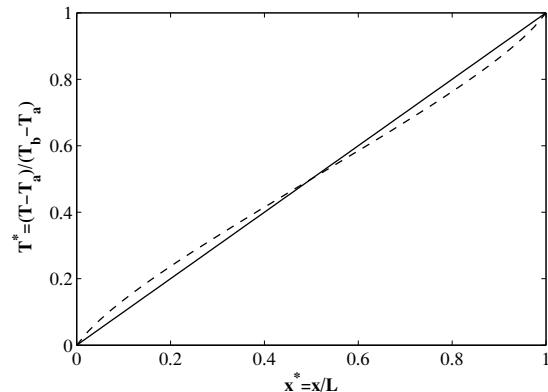


Figure 3. Steady-state dimensionless temperature field for a fractional bar with $\alpha = 1.5$ (dashed line) and $\alpha = 2$ (continuous line).

3.2. Steady-state solution

In the steady-state regime Eq. (6) reverts to:

$$\frac{kc_\alpha}{2} \{ {}^C D_{a+}^\alpha [T(x) - T(a)] + {}^C D_{b-}^\alpha [T(x) - T(b)] \} = -S(x). \quad (14)$$

By supposing that the temperatures at the ends of the bar are different, $T_b > T_a$, the dimensionless temperature can now be defined as $T^* = (T - T_a)/(T_b - T_a)$. The value for the parameter c_α^* is the same as above. According to the classical case ($\alpha = 2$), the temperature field in the steady-state regime would be linear and equal to $T^*(x^*) = x^*$. On the other hand, as can be evinced from Fig. 3 the fractional solution becomes non-linear, this effect becoming more pronounced as α decreases. Moreover, the gradient of the temperature concentrates at the bar extremes (Fig. 4). This effect can be explained by noting that the zones close to the borders conduct less because of lower presence of the long-range interactions.

Let us now give a physical interpretation to fractional operators. Notice that Eq. (14) can be expressed through the Caputo fractional derivatives [27]

$$\frac{kc_\alpha}{2} \{ {}^C D_{a+}^\alpha [T(x)] + {}^C D_{b-}^\alpha [T(x)] \} = -S(x) \quad (15)$$

which can be rewritten, for sufficiently regular functions, by exploiting the definition of the Marchaud fractional derivatives (Eqs. (5A) and (6A), [36]), as:

$$\begin{aligned} \frac{kc_\alpha}{2} \frac{(\alpha - 1)}{\Gamma(2 - \alpha)} \left[\frac{T(x) - T(a)}{(x - a)^\alpha} + \frac{T(x) - T(b)}{(b - x)^\alpha} \right. \\ \left. + \alpha \int_a^b \frac{T(x) - T(y)}{|x - y|^{1+\alpha}} dy \right] = S(x). \end{aligned} \quad (16)$$

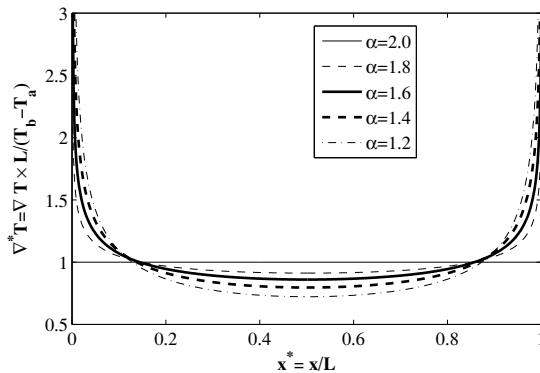


Figure 4. Steady-state dimensionless temperature-gradient fields for fractional bars with different orders α .

For the inner points of the domain ($i = 2, \dots, n$), the discrete form of Eq. (16) reads:

$$k_{i,1}^{vs}(T_i - T_1) + k_{i,n+1}^{vs}(T_i - T_{n+1}) + \sum_{j=1, j \neq i}^{n+1} k_{i,j}^{vv}(T_i - T_j) = S_i A \Delta x, \quad (17)$$

where A is the cross-sectional area. It is evident how the nonlocal fractional model is equivalent to a point-conductor model where two kinds of conductors appear: the former connecting the inner material points with the bar edges, ruling the volume-surface long-range interactions, with conductance k^{vs} ; the latter connecting the inner material points each other, describing the nonlocal interactions between non-adjacent volumes, whose conductance is k^{vv} . Provided that the indexes are never equal one to the other, the following expressions for the conductance hold ($i = 1, \dots, n+1$):

$$k_{i,1}^{vs} = k_{1,i}^{vs} = \frac{kc_\alpha}{2} \frac{\alpha - 1}{\Gamma(2 - \alpha)} \frac{A \Delta x}{(x_i - x_1)^\alpha}, \quad (18)$$

$$k_{i,n+1}^{vs} = k_{n+1,i}^{vs} = \frac{kc_\alpha}{2} \frac{\alpha - 1}{\Gamma(2 - \alpha)} \frac{A \Delta x}{(x_{n+1} - x_i)^\alpha}, \quad (19)$$

$$k_{i,j}^{vv} = k_{j,i}^{vv} = \frac{kc_\alpha}{2} \frac{\alpha(\alpha - 1)}{\Gamma(2 - \alpha)} \frac{A(\Delta x)^2}{|x_i - x_j|^{1+\alpha}}. \quad (20)$$

Furthermore, by looking at the boundary boundary condition (10), it is possible to state that a fourth set of conductors has to be introduced: it is composed by a unique conductor connecting the two bar extremes with conductance

$$k_{1,n+1}^{ss} = k_{n+1,1}^{ss} = \frac{kc_\alpha}{2 \Gamma(2 - \alpha)} \frac{A}{(x_{n+1} - x_1)^{\alpha-1}}. \quad (21)$$

The superscript ss for the conductance (21) is used since the element connecting the bar edges can be seen as modelling the interactions between material points lying on the surface, which, in the simple one-dimensional model under examination, reduce to the two points $x = a, b$. Note that the presence of such a conductor was implicitly embedded in the constitutive equation (3). However, since it provides a constant heat flux contribution throughout the bar length, its presence was lost by derivation when passing from Eq. (3) to Eq. (6).

To summarize, the constitutive fractional relationship (3) is equivalent to a point-conductor model with three sets of nonlocal conductors (17)–(21). Note that their conductances all decay with the distance, although the decaying velocity differs from one kind to the other.

4. Conclusions

In the present work, diffusion processes in nonlocal unidimensional media, i.e. solids characterized by nonlocal interactions, are investigated. The proposed approach is based on fractional calculus, which deals with integrals and derivatives of generic order: fractional operators replace the classical ones in the governing equation. The model results to be original with respect to many points: i) the nonlocal fractional differential equation is consistently derived starting from the conservation of the internal energy. Suitable boundary conditions are also specified; ii) the problem is set on a finite domain and solved by means of fractional finite differences; iii) a physically-sound interpretation of fractional operators has been derived.

Acknowledgements

The financial supports of the Italian Ministry of Education, University and Research (MIUR) to the Project FIRB 2010 Future in Research 'Structural mechanical models for renewable energy applications' are gratefully acknowledged.

Appendix

The most frequently used definitions of fractional integral of order β ($\beta \in \mathbb{R}^+$) are due to Riemann-Liouville and represent a straightforward generalization to non-integer values of Cauchy formula for repeated integrations. The left and right Riemann-Liouville fractional integrals read,

respectively:

$$I_{a+}^\beta f(x) = \frac{1}{\Gamma(\beta)} \int_a^x \frac{f(y)}{(x-y)^{1-\beta}} dy, \quad (1A)$$

$$I_{b-}^\beta f(x) = \frac{1}{\Gamma(\beta)} \int_x^b \frac{f(y)}{(y-x)^{1-\beta}} dy. \quad (2A)$$

On the other hand, the Riemann-Liouville fractional derivatives are defined as the derivatives of order n ($n \in \mathbb{N}$ and $n-1 < \beta < n$, [35]) of the fractional integral of order $(n-\beta)$:

$$D_{a+}^\beta f(x) = \frac{d^n}{dx^n} I_{a+}^{n-\beta} f(x), \quad (3A)$$

$$D_{b-}^\beta f(x) = -\frac{d^n}{dx^n} I_{b-}^{n-\beta} f(x). \quad (4A)$$

As proved in [36], 'for sufficiently good functions', Eqs. (3A) and (4A) revert to

$$\begin{aligned} D_{a+}^\beta f(x) &= \sum_{k=0}^{n-1} \frac{f^k(a)}{\Gamma(1+k-\beta)} (x-a)^{k-\beta} \\ &\quad + \frac{1}{\Gamma(n-\beta)} \int_a^x \frac{f^n(y)}{(x-y)^{\beta-n+1}} dy, \end{aligned} \quad (5A)$$

$$\begin{aligned} D_{b-}^\beta f(x) &= \sum_{k=0}^{n-1} \frac{(-1)^k f^k(b)}{\Gamma(1+k-\beta)} (b-x)^{k-\beta} \\ &\quad + \frac{(-1)^n}{\Gamma(n-\beta)} \int_x^b \frac{f^n(y)}{(y-x)^{\beta-n+1}} dy, \end{aligned} \quad (6A)$$

which coincide with the Marchaud's definitions of fractional derivatives.

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