On the Solution of Time-Fractional Diffusion Models

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Abstract. In many situations, the analysis of viscoelastic materials, like polymers, takes benefit from the introduction of fractional operators in the mathematical formalization. In addition, fractional differential models have been applied in a wide variety of fields, from biology to thermodynamics, from diffusion of information to dehydration/rehydration of food. Thus, a great interest is paid both in the analytical and in the numerical solution of fractional differential problems. The present paper considers a class of time-fractional diffusion problems with Dirichlet boundary conditions. Using Duhamel's principle, the analytical solution is found. As usual in this context, the solution is given in series form and depends on the Mittag-Leffler function. We suggest a computational procedure to evaluate the solution with high accuracy, in a computing environment. Some test examples are presented both in the subdiffusion and in the superdiffusion case, to illustrate the behavior of the solution for different values of the fractional index. Test cases have been carried out in MATLAB.

Keywords: Anomalous diffusion · Fractional differential equations · Analytical solution · Dirichlet boundary conditions

1 Introduction

The modelling of materials by fractional calculus leads to an accurate description of the experimental data and to reliable predictions of the phenomena in many cases where classical models provide unsatisfactory results. As a matter of fact, the fractional derivative of a function, depends on its past history, therefore fractional operators are specially suitable to model phenomena with memory. Typical examples of fractional models regard viscoelastic materials, which have a hereditary nature, like polymers, epoxy resins, fruit and vegetables (compare [13,14,18,28,30] and references therein). Another field where the memory effects may be well described by fractional operators is heat conduction, giving rise to fractional thermo-elasticity [32], fractional thermo-viscoelasticity [36], fractional electro-thermoelasticity [17]. A special mention is also due to the heat conduction near a crack [40]. The anomalous diffusion, which is observed in many

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processes and in particular in the transport through heterogeneous media, is well described by fractional models. In particular, time-fractional operators are able to catch the slow decay of initial conditions and memory effects in subdiffusion of complex systems, like proteins (see references cited in [1]). Anomalous diffusion is observed in dehydration and rehydration processes of food [24,37], in the diffusion of drugs through skin, in the atrial tissue [35]. Moreover, the anomalous diffusion and its fractional modelling have been considered also in other situations, like the diffusion of information in social networks [20].

The great interest towards the fractional diffusion models led to the development of both analytical and numerical tools. Some important references on the analytical solutions are [2,25,26,34,39]. A wide literature is available in the numerical approximation, by linear multistep methods, collocation methods, spectral methods and many other approaches [1,3–12,15,16,19,22,29,41].

In this paper, we provide the analytical solution of the time-fractional diffusion equation

$$D_t^\alpha u = c u_{xx}, \qquad p-1 < \alpha < p, \qquad x \in [0, L], \qquad t \geq 0, \qquad p \in \mathbb{N} \tag{1}$$

where c is a constant diffusion coefficient, with null initial conditions, and Dirichlet boundary conditions:

$$D_t^k u(x,0) = 0, \qquad k = 0, \ldots, p-1, \qquad u(0,t) = \gamma_0(t), \qquad u(L,t) = \gamma_1(t). \tag{2}$$

Here D_t^α is the fractional derivative, in the Riemann-Liouville or in the Caputo sense [31]. Equations of type (1) cover a general class of problems, e.g. [20,24,33,37,40]. The solution u may represent the temperature field in heat conduction or the concentration of a substance in diffusion processes. Some existence and uniqueness results, for the subdiffusion case $0 < \alpha < 1$, may be found in [2,25,26]. For the theory on the more general case $0 < \alpha < 2$, compare [27] and references therein.

We derive the analytical solution by means of Duhamel's principle [34,38,39]. Although the solution is given in a series form, it may be accurately evaluated in common computing environments, like Mathematica, MATLAB or Python, thanks to a suitable truncation of the series, as we will show in the numerical examples. Secondly, any a priori knowledge on the analytical solution is a fundamental starting point to obtain reliable and efficient numerical methods, by suggesting the function basis to approximate the solution.

The paper is organized as follows. Some basic notions on fractional calculus are included in Sect. 2. In Sect. 3 we derive the analytical solution of problem (1)–(2). In Sect. 4 we show some examples of solutions in the subdiffusion and superdiffusion case.

2 Basic Mathematic Material

In this section we introduce some preliminary material on fractional calculus. For further details compare [31]. Fractional differential equations are defined by

establishing a relation between a function and its fractional derivatives (that can also be the standard derivatives of integer order).

The definition of fractional derivative is not unique. The most popular ones are the Riemann-Liouville fractional derivative,

$$ {}^{\mathrm{RL}}D_t^\alpha f = D_t^p(I_t^{p-\alpha} f), \tag{3}$$

and the Caputo fractional derivative,

$$ D_t^\alpha f = I_t^{p-\alpha}(D_t^p(f)), \tag{4}$$

where in both cases,

$$ I_t^{p-\alpha} f = \frac{1}{\Gamma(p-\alpha)} \int_0^t \frac{f(\tau, x)}{(t-\tau)^{1-p+\alpha}} \, \mathrm{d}\tau \tag{5}$$

is the Riemann-Liouville integral and $\Gamma(z)$ is the Gamma function.

The two definitions (3) and (4) are related by

$$ D_t^\alpha f = {}^{\mathrm{RL}}D_t^\alpha f - {}^{\mathrm{RL}}D_t^\alpha \left(\sum_{k=0}^{p-1} \frac{t^k}{k!} f^{(k)}(0) \right), \tag{6}$$

and so they coincide if and only if the function f is such that

$$ f^{(k)}(0) = 0, \qquad k = 0, \ldots, p-1. $$

In the field of Ordinary Differential Equations (ODEs), the exponential function $y(z) = \mathrm{e}^z$ solves the problem

$$ y'(z) = y(z), \qquad y(0) = 1. $$

In the context of fractional ODEs, the solution of the analogue problem

$$ D_z^\alpha y(z) = y(z), \qquad y(0) = 1, $$

is $E_\alpha(t^\alpha)$, where E_α is known as the Mittag-Leffler function, defined as

$$ E_\alpha(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + 1)}. $$

Note that, as expected, $E_1(z) = \mathrm{e}^z$, so the Mittag-Leffler function can be seen as a generalization of the exponential function.

A further generalization is the Mittag-Leffler function with two arguments,

$$ E_{\alpha,\beta}(z) = \sum_{k=0}^{\infty} \frac{z^k}{\Gamma(\alpha k + \beta)}. \tag{7}$$

Setting $\beta = 1$, the function (7) reduces to the Mittag-Leffler function with one argument, i.e., $E_\alpha = E_{\alpha,1}$.

In the next sections we will make use of the following relations that hold true for any $\alpha > 0$, $\beta > 0$, k integer, and γ and λ real numbers [31]

$$ {}^{\mathrm{RL}}D_t^{\gamma}\left(t^{\alpha k+\beta-1}E_{\alpha,\beta}^{(k)}(\lambda t^{\alpha})\right) = t^{\alpha k+\beta-\gamma-1}E_{\alpha,\beta-\gamma}^{(k)}(\lambda t^{\alpha}), \tag{8} $$

$$ \int_0^t (t-\tau)^{\gamma-1}E_{\alpha,\beta}(\lambda\tau^{\alpha})\tau^{\beta-1}\,\mathrm{d}\tau = \Gamma(\gamma)t^{\beta+\gamma-1}E_{\alpha,\beta+\gamma}(\lambda t^{\alpha}). \tag{9} $$

3 The Solution of the Time-Fractional Diffusion Problem

We consider the time-fractional diffusion equation (1) with initial and boundary conditions (2).

We assume that the initial data and the boundary conditions are compatible, and therefore

$$ D_t^k\gamma_0(0) = D_t^k\gamma_1(0) = 0, \qquad k = 0,\ldots,p-1. \tag{10} $$

The symbol D_t^{α} denotes here the Caputo fractional derivative. However, as the initial condition is of total rest, for this problem this is equivalent to the Riemann-Liouville fractional derivative.

We introduce the auxiliary function

$$ h(x,t) = \frac{x}{L}(\gamma_0(t)-\gamma_1(t)) - \gamma_0(t). \tag{11} $$

The variable

$$ v(x,t) = u(x,t) + h(x,t) \tag{12} $$

is the solution of

$$ D_t^{\alpha}v = cv_{xx} + D_t^{\alpha}h \tag{13} $$

that satisfies zero initial and boundary conditions,

$$ D_t^k v(x,0) = 0, \qquad k = 0,\ldots,p-1, \qquad v(0,t) = 0, \qquad v(L,t) = 0, \tag{14} $$

as a consequence of (10) and (11). We assume that the boundary conditions are regular enough such that h there exists

$$ \varphi(x,t) = D_t^p h(x,t). \tag{15} $$

Then,

$$ D_t^{\alpha}h = I_t^{p-\alpha}\varphi(x,t). $$

Note that this fractional derivative can be computed as h is known.

In order to find v, we recur to the following fractional Duhamel's principle.

Theorem 1 (Duhamel's principle [34,38,39]**).** *Let be $w(x,t)$ the solution of the unforced fractional problem*

$$ D_t^{\alpha}w(x,t;\tau) = cw_{xx}(x,t;\tau), \tag{16} $$

with initial and boundary conditions

$$D_t^k w(x,0;\tau)=0,\quad k=0,\dots,p-1,\qquad D_t^{p-1}w(x,0;\tau)=\varphi(x,\tau),$$
$$w(0,t;\tau)=w(L,t;\tau)=0. \tag{17}$$

The solution of the forced problem (13) *with homogeneous initial and boundary conditions* (14) *is*

$$v(x,t)=\int_0^t w(x,t-\tau;\tau)\,\mathrm{d}\tau, \tag{18}$$

The following theorem gives the solution of problem (16)–(17) in closed form for any fractional value of α.

Theorem 2. *The solution of problem* (16)–(17) *is*

$$w(x,t;\tau)=\sum_{n=1}^{\infty} t^{p-1}\varphi_n(\tau)E_{\alpha,p}(-c\lambda_n^2 t^\alpha)\sin(\lambda_n x), \tag{19}$$

where $\lambda_n=n\pi/L$, *and* $\varphi_n(t)$ *is the n-th coefficient of the sine-expansion of* $\varphi(x,t)$ *in space,*

$$\varphi_n(t)=\frac{2}{L}\int_0^L \varphi(x,t)\sin(\lambda_n x)\,\mathrm{d}x. \tag{20}$$

Proof. Evaluating $w(x,t;\tau)$ *at* $x=0$ *and* $x=L$, *we immediately find that the boundary conditions in* (17) *are satisfied.*

Considering that

$$D_t^k(t^{p-1}E_{\alpha,p}(-c\lambda_n^2 t^\alpha))=\sum_{j=0}^{k}\binom{k}{j}D_t^j t^{p-1}D_t^{k-j}E_{\alpha,p}(-c\lambda_n^2 t^\alpha),$$

then

$$D_t^k(t^{p-1}E_{\alpha,p}(-c\lambda_n^2 t^\alpha))\big|_{t=0}=0,\qquad k=0,\dots,p-2, \tag{21}$$
$$D_t^{p-1}(t^{p-1}E_{\alpha,p}(-c\lambda_n^2 t^\alpha))\big|_{t=0}=(p-1)!E_{\alpha,p}(0)=1. \tag{22}$$

Therefore,

$$D_t^k w(x,0;\tau)=\sum_{n=1}^{\infty}\varphi_n(\tau)\sin(\lambda_n x)D_t^k(t^{p-1}E_{\alpha,p}(-c\lambda_n^2 t^\alpha))\big|_{t=0}=0,$$

for $k=0,\dots,p-2$, *and*

$$D_t^{p-1}w(x,0;\tau)=\sum_{n=1}^{\infty}\varphi_n(\tau)\sin(\lambda_n x)D_t^{p-1}(t^{p-1}E_{\alpha,p}(-c\lambda_n^2 t^\alpha))\big|_{t=0}$$
$$=\sum_{n=1}^{\infty}\varphi_n(\tau)\sin(\lambda_n x)=\varphi(\tau).$$

Hence, $w(x,t;\tau)$ satisfies also the initial conditions in (17).

Finally, we evaluate

$$w_{xx}(x,t;\tau) = -\sum_{n=1}^{\infty} \lambda_n^2 t^{p-1} \varphi_n(\tau) E_{\alpha,p}(-c\lambda_n^2 t^\alpha) \sin(\lambda_n x),$$

and

$$D_t^\alpha w(x,t;\tau) = \sum_{n=1}^{\infty} \varphi_n(\tau) \sin(\lambda_n x) D_t^\alpha (t^{p-1} E_{\alpha,p}(-\lambda_n^2 t^\alpha)). \tag{23}$$

Considering Eq. (6) and substituting (21) and (22), Eq. (23) is equivalent to

$$\begin{aligned} D_t^\alpha w(x,t;\tau) &= \sum_{n=1}^{\infty} \varphi_n(\tau) \sin(\lambda_n x) \left({}^{RL}D_t^\alpha (t^{p-1} E_{\alpha,p}(-c\lambda_n^2 t^\alpha)) - {}^{RL}D_t^\alpha \left(\frac{t^{p-1}}{(p-1)!} \right) \right) \\ &= \sum_{n=1}^{\infty} \varphi_n(\tau) \sin(\lambda_n x) \left({}^{RL}D_t^\alpha (t^{p-1} E_{\alpha,p}(-c\lambda_n^2 t^\alpha)) - \frac{t^{p-1-\alpha}}{\Gamma(p-\alpha)} \right). \end{aligned} \tag{24}$$

Moreover, applying formula (8) with $k=0$, $\gamma=\alpha$, $\beta=p$, and $\lambda=-c\lambda_n^2$, yields

$$\begin{aligned} {}^{RL}D_t^\alpha (t^{p-1} E_{\alpha,p}(-c\lambda_n^2 t^\alpha)) &= t^{p-\alpha-1} E_{\alpha,p-\alpha}(-c\lambda_n^2 t^\alpha) = t^{p-\alpha-1} \sum_{k=0}^{\infty} \frac{(-c\lambda_n^2 t^\alpha)^k}{\Gamma(\alpha(k-1)+p)} \\ &= -c\lambda_n^2 t^{p-1} \sum_{k=0}^{\infty} \frac{(-c\lambda_n^2 t^\alpha)^{k-1}}{\Gamma(\alpha(k-1)+p)} \\ &= -c\lambda_n^2 t^{p-1} \left(\frac{1}{(-c\lambda_n^2 t^\alpha)\Gamma(p-\alpha)} + \sum_{k=0}^{\infty} \frac{(-c\lambda_n^2 t^\alpha)^k}{\Gamma(\alpha k+p)} \right) \\ &= \frac{t^{p-1-\alpha}}{\Gamma(p-\alpha)} - c\lambda_n^2 t^{p-1} E_{\alpha,p}(-c\lambda_n^2 t^\alpha). \end{aligned}$$

Substituting in formula (24), gives

$$D_t^\alpha w(x,t;\tau) = -c \sum_{n=1}^{\infty} \lambda_n^2 t^{p-1} \varphi_n(\tau) E_{\alpha,p}(-c\lambda_n^2 t^\alpha) \sin(\lambda_n x) = c w_{xx}(x,t;\tau),$$

that completes the proof.

Theorem 3. *The solution of problem (1)–(2) is*

$$u(x,t) = \int_0^t \sum_{n=1}^{\infty} (t-\tau)^{p-1} \varphi_n(\tau) E_{\alpha,p}(-c\lambda_n^2 (t-\tau)^\alpha) \sin(\lambda_n x)\, \mathrm{d}\tau - h(x,t), \tag{25}$$

where φ_n has been defined in (20).

Proof. According to Theorem 1, the solution $v(x,t)$ of problem (13)–(14) is obtained by evaluating $w(x,t-\tau;\tau)$ and substituting in (18). Substituting $v(x,t)$ in (12), we obtain that the solution of (1)–(2) is given by (25).

4 Test Examples

We propose here numerical results for some of the most popular examples of anomalous diffusion modelled by Eq. (1), that are those of subdiffusion, i.e. $0 < \alpha < 1$, and of superdiffusion with $1 < \alpha < 2$. We used MATLAB R2020a to compute and plot the solution.

In order to reproduce numerical results, we need first to set up a grid of nodes on which the solutions are evaluated. We denote with $\mathbf{x}$ and $\mathbf{t}$ the vectors of the nodes in space and time, respectively, i.e.:

$$x_m = m\Delta x,\ m = 0, \ldots, M, \quad t_j = j\Delta t,\ j = 0, \ldots, J,$$

$\Delta x = L/M$, $\Delta t = T/J$.

All the analytical solutions obtained in this paper are in the form of a series:

$$\sum_{n=1}^{\infty} a_n(x,t).$$

Thus, the infinite sum needs to be truncated. The solution at the grid nodes is approximated as

$$\sum_{n=1}^{N} a_n(\mathbf{x},\mathbf{t}), \tag{26}$$

where $a_n(\mathbf{x},\mathbf{t})$ is the matrix of the values of a_n at the grid points, and N is the smallest integer such that $\|a_N(\mathbf{x},\mathbf{t})\| < \text{tol} = 10^{-12}$, with $\|\cdot\|$ denoting the spectral norm, i.e.,

$$\|a_N\| = \sqrt{\lambda_{\max}},$$

and $\lambda_{\max}$ is the maximum eigenvalue of the matrix $a_N^T a_N$.

Secondly, we computed the Mittag-Leffler function by the MATLAB routine `ml` [21,23].

Subdiffusion

Let us consider Eq. (1) with $0 < \alpha < 1$, $c = 1$, $(x,t) \in (0,1) \times (0,2)$, and boundary conditions,

$$u(0,t) = u(1,t) = t.$$

Therefore, Eq. (11) and (15), yield

$$h(x,t) = -t,$$

and

$$\varphi(x,t) = D_t h(x,t) = -1,$$

respectively. Moreover,

$$\varphi_n(t) = -\frac{2}{L}\int_0^L \sin(\lambda_n x)\,\mathrm{d}x = \frac{2((-1)^n - 1)}{n\pi}, \tag{27}$$

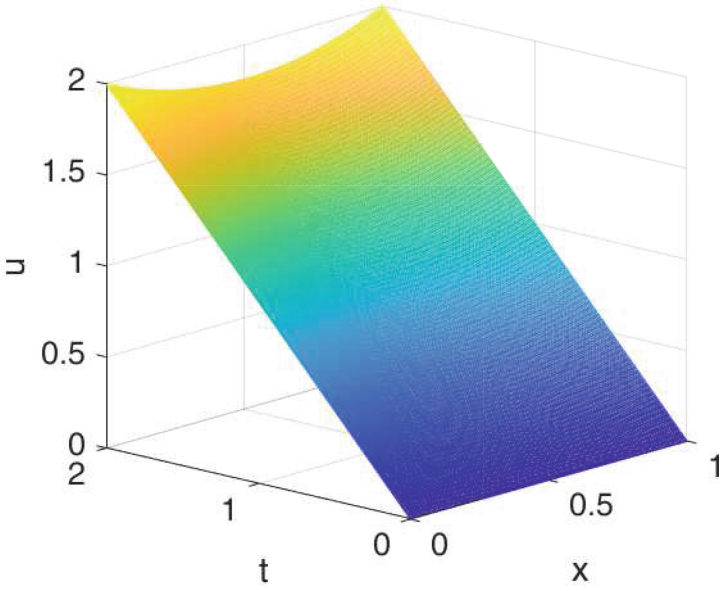

Fig. 1. Solution of the subdiffusion problem with $\alpha = 0.5$.

and since for n even $\varphi_n = 0$, the solution (25) reduces to

$$\begin{aligned} u(x,t) &= \int_0^t \sum_{n=1}^{\infty} \frac{-4}{(2n-1)\pi} E_\alpha(-\lambda_{2n-1}^2 (t-\tau)^\alpha) \sin(\lambda_{2n-1} x)\, \mathrm{d}\tau + t \\ &= \sum_{n=1}^{\infty} \frac{-4}{(2n-1)\pi} \sin(\lambda_{2n-1} x) \int_0^t E_\alpha(-\lambda_{2n-1}^2 \tau^\alpha)\, \mathrm{d}\tau + t \\ &= \sum_{n=1}^{\infty} \frac{-4t}{(2n-1)\pi} \sin(\lambda_{2n-1} x) E_{\alpha,2}(-\lambda_{2n-1}^2 t^\alpha) + t \end{aligned}$$

where, after a change of variable, we have used formula (9) with $\beta = \gamma = 1$ and $\lambda = -\lambda_{2n-1}^2$.

In Fig. 1 we show, as an example, the solution obtained with the intermediate value $\alpha = 0.5$ and evaluated on a grid with 200 equispaced nodes in space and 100 equispaced points in time. The infinite sum is truncated according to (26), and in this case $N = 12232$. It is visible that starting from a configuration of rest, the heat/substance spreads more uniformly at the beginning, whereas for larger times the temperature/amount of substance is visibly higher at the boundary and lower at the center.

In Fig. 2 we compare the solutions obtained for different values of α uniformly spread in the interval $(0, 1)$. Note that when $\alpha = 0$, problem (1)–(2) reduces to a boundary value problem for an ODE. The results obtained highlight that for any fractional value of α corresponds an intermediate configuration of the solution

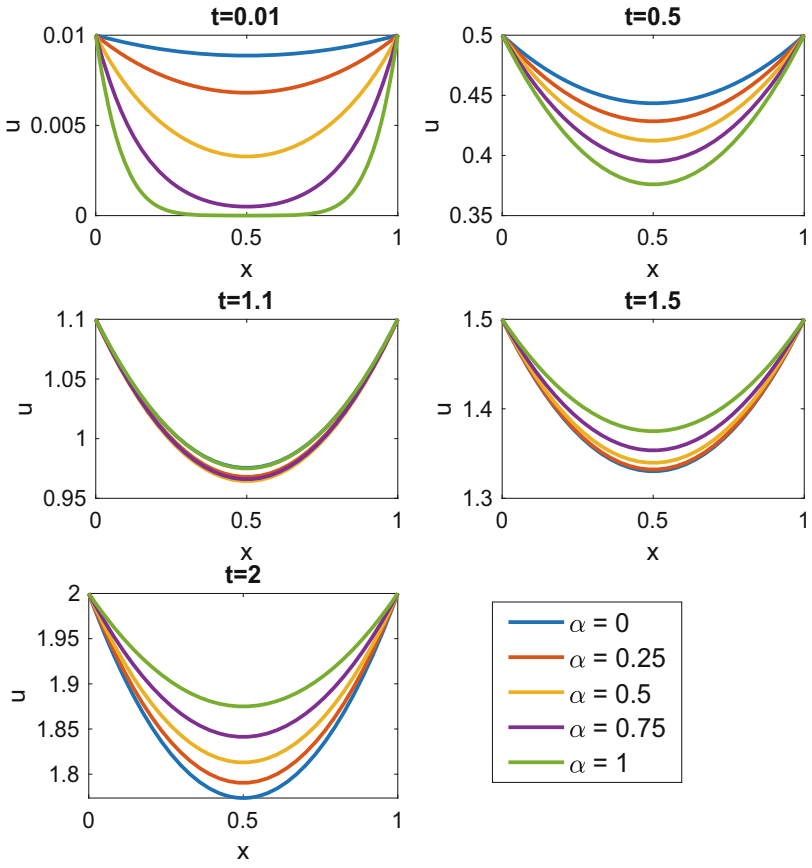

Fig. 2. Subdiffusion problem: Solution for different values of α at different times.

between those obtained in the two integer cases, $\alpha = 0$ and $\alpha = 1$. These two extreme configurations are approached continuously and monotonically as α approaches 0 or 1, respectively.

The comparisons show that at the beginning the diffusion from the boundary source to the center of the one dimensional domain is faster for smaller values of α. However, there exists a critical time, around $t = 1.1$ where this trend is inverted. After this time, the spread is faster for higher values of α.

Superdiffusion

We consider now Eq. (1) with $1 < \alpha < 2$, again with $c = 1$, $(x, t) \in (0, 1) \times (0, 2)$ and boundary conditions,

$$u(0, t) = u(1, t) = \frac{t^2}{2}.$$

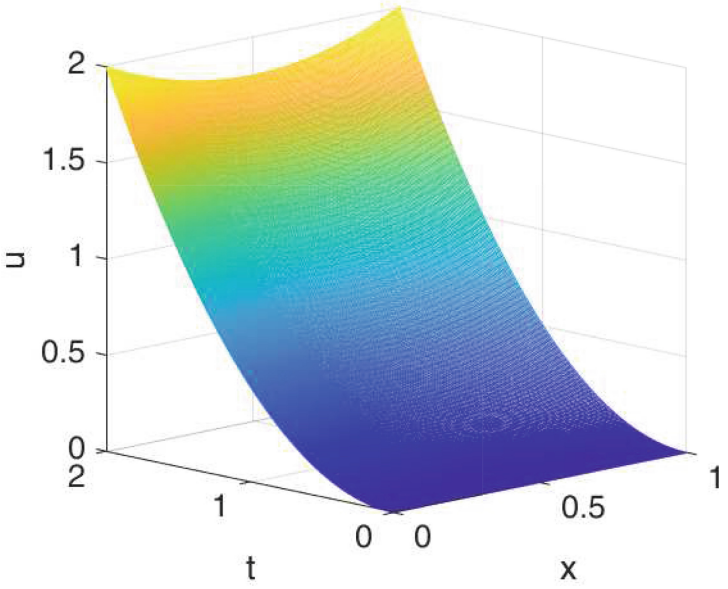

Fig. 3. Solution of the superdiffusion problem with $\alpha = 1.5$.

Therefore,

$$h(x,t) = -\frac{t^2}{2},$$

and

$$\varphi(x,t) = D_t^2 h(x,t) = -1,$$

so, also in this case, the coefficients φ_n are defined by Eq. (27). Substituting in Eq. (25), gives the following infinite expansion of the solution:

$$\begin{aligned} u(x,t) &= \int_0^t \sum_{n=1}^{\infty} \frac{-4(t-\tau)}{(2n-1)\pi} E_{\alpha,2}(-\lambda_{2n-1}^2 (t-\tau)^\alpha) \sin(\lambda_{2n-1} x)\, \mathrm{d}\tau + \frac{t^2}{2} \\ &= \sum_{n=1}^{\infty} \frac{-4}{(2n-1)\pi} \sin(\lambda_{2n-1} x) \int_0^t \tau E_{\alpha,2}(-\lambda_{2n-1}^2 \tau^\alpha)\, \mathrm{d}\tau + \frac{t^2}{2}, \\ &= \sum_{n=1}^{\infty} \frac{-4t^2}{(2n-1)\pi} \sin(\lambda_{2n-1} x) E_{\alpha,3}(-\lambda_{2n-1}^2 t^\alpha) + \frac{t^2}{2}, \end{aligned}$$

where we have used (9) with $\gamma = 1$, $\beta = 2$ and $\lambda = -\lambda_{2n-1}$.

As an example, we consider the solution obtained with $\alpha = 1.5$ and truncate the infinite sum after the first $N = 12232$ terms (also in this case the next terms are smaller than the chosen tolerance value). A graph of the solution on the same grid of Fig. 1 is shown in Fig. 3. Similarly as in the case of subdiffusion, starting with an initial condition of total rest the diffusion is more uniform along

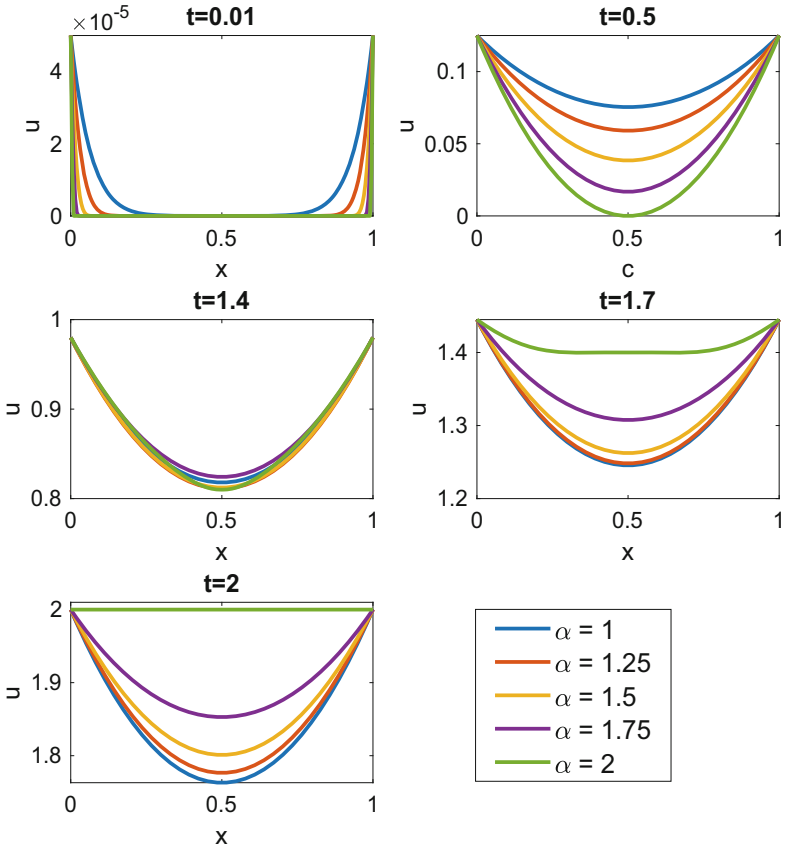

Fig. 4. Subdiffusion problem: Solution for different values of α at different times.

the domain for the smallest values of t, whereas a clear difference between the boundary and the center is visible for larger values of the boundary source as time increases.

In Fig. 4 we compare the solutions obtained with different values of α chosen uniformly in the interval $(1, 2)$. When $\alpha = 1$, the problem is solved imposing a single initial condition $u(x, 0) = 0$.

As before, the solutions obtained for non integer values of $\alpha \in (1, 2)$ have a configuration that is always intermediate between that of the solutions of the PDEs of integer order. These are approached smoothly for α tending to 1 or to 2, respectively.

At the beginning the diffusion is very slow for the largest values of α, and faster as α approaches 1. After a critical time, around $t = 1.4$, this trend is inverted and the diffusion from the boundary source toward the center is faster for higher values of α.

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