Fractional Diffusion Problems with Reflecting Boundaries

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Abstract. Anomalous diffusive transport, described by fractional differential equations, arises in a large variety of physical problems. We consider a fractional diffusion equation subjected to reflecting boundary conditions. The formulation of these boundaries has sparked a controversial discussion, with questions arising about the most appropriate boundary from the physical point of view. Therefore, we start to present different physical formulations regarding the boundaries. Numerical methods are then proposed to solve these diffusive models, and it is shown how the presence of boundaries changes the general structure of the problem and of the numerical method, due to the non-locality of the problem. In the end, the impact of the different boundaries on the solutions is analysed.

1 Introduction

Anomalous diffusive transport related to Lévy flights can be formulated via fractional differential equations [10]. It frequently happens that we have to apply boundary conditions when considering experimental devices and attempting to check a model for mass transport in a given medium. Due to non-locality, it is not obvious how to incorporate a boundary condition in a scenario based on Lévy flights, since the long jumps pose certain difficulties when boundary conditions are involved. In fact, the presence of certain boundaries modifies the nonlocal spatial operator since they cannot be uncoupled from the fractional partial differential equation. In literature, when discussing Lévy flights in the one dimensional half-space the boundary conditions mainly considered have been absorbing or reflecting boundaries. Absorbing boundary conditions have been imposed by assuming zero outside the problem domain. However, regarding reflecting boundary conditions several formulations have been proposed [1,3–9].

The proper formulation of physically meaningful reflecting boundary conditions for fractional diffusion equations requires careful consideration of the nonlocal operator. In this work we discuss two types of boundaries that appear respectively in [9] and [2], showing the impact of both formulations on the numerical method and on the solution. In [9] the influence of a reflective wall is modelled within the framework of space-time fractional partial differential equations. The jumps do not interact with the wall and they are as in a free space. This is modelled by a fractional differential equation that involves a non-local operator which kernel takes into account the boundary condition. In [2] the physical

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boundary conditions are derived using a mass balance approach and the reflecting boundary condition is formulated in terms of a fractional derivative.

2 The Models

The diffusive model associated to Lévy flights is defined in the whole real line and the governing equation involves Riemann-Liouville fractional derivatives [10]. We consider the assymetric case, that is, the diffusive operator is defined only with the left Riemann-Liouville fractional derivative.

2.1 Open Domain

We start with the open domain and then describe how to evolve to the situation of having a reflecting boundary condition.

The left Riemann-Liouville fractional derivative of order α, when $1 < \alpha < 2$, for $x \in \mathbb{R}$, is given by

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x,t) = \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_{-\infty}^{x} u(\xi,t)(x-\xi)^{1-\alpha}d\xi. \tag{1}$$

The fractional differential equation describing the diffusive model under consideration in the open domain, for $1 < \alpha < 2$, can be stated as

$$\frac{\partial u(x,t)}{\partial t} = D\frac{\partial^\alpha u}{\partial x^\alpha}(x,t), \tag{2}$$

where D is the diffusive parameter and the parameter α is related to the tail of the solution. In this scenario of having an open domain we assume that we have an initial condition $u(x,0) = u_0(x),\ x \in \mathbb{R}$, and that the solution goes to zero when $|x|$ goes to infinity.

In the next sections, we describe how this problem changes in the presence of a boundary at $x = 0$ and defined in the domain $x > 0$.

2.2 The Symmetric Boundary Wall

In this section we present how to formulate the diffusive problem with a left reflecting wall. The formulation of the boundary is according to [9], where a symmetric diffusive problem on a semi-infinite domain is considered. Physically, when considering a trajectory of the particle in $[0,\infty)$ with the reflecting boundary condition at $x = 0$, the jumps that end at $x < 0$ are reflected. Therefore, the model under study consists on a reflecting wall restraining the diffusing particles to a semi-infinite domain. This barrier can be viewed as a force field applied to the particles. It is assumed that the particles arriving at the boundary are bounced back as in elastic collisions, that is, if they reach the position $x = -a$ with $a > 0$, then they will end at $x = a$, describing the mirror trajectory with respect to the wall. In a porous medium such a boundary may represent a wall permeable to the fluid, but impermeable to the tracer. Mathematically, we have a problem defined in $x > 0$ by Eq. (2) and subjected to the wall condition, $u(x,t) = u(-x,t)$, for $x < 0$. Taking in consideration this wall condition, the left Riemann-Liouville fractional derivative (1) becomes a different operator, for $x > 0$, that we define as the reflecting left Riemann-Liouville fractional derivative,

$$\begin{aligned}\frac{\partial^{\alpha}_{ref} u}{\partial x^{\alpha}}(x,t) :=& \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_0^{\infty} u(\xi,t)(x+\xi)^{1-\alpha} d\xi \\ &+ \frac{1}{\Gamma(2-\alpha)}\frac{\partial^2}{\partial x^2}\int_0^{x} u(\xi,t)(x-\xi)^{1-\alpha} d\xi. \end{aligned} \quad (3)$$

Formally when subjected to a reflecting wall we have the following problem,

$$\frac{\partial u}{\partial t}(x,t) = D\frac{\partial^{\alpha}_{ref} u}{\partial x^{\alpha}}(x,t), \quad x > 0, \quad (4)$$

$$u(x,t) = u(-x,t), \quad \text{for all} \quad x < 0, \quad (5)$$

with an initial condition $u(x,0) = u_0(x)$, $x \geq 0$.

2.3 A Fractional Boundary Condition

Consider the boundary condition as defined in [2], that involves a fractional derivative of order $\alpha - 1$. The physical setup is described as having mass concentration resting at the boundary instead of having mass leaving the domain. This means mass is preserved, and moved to the boundary. Unlike the traditional diffusion setup, this mass can come from far inside the domain, not just an adjacent grid point.

Let us define the fractional derivative of order $m - 1 < \alpha < m$, starting at $x = 0$, by

$$\frac{\partial^{\alpha}_{0} u}{\partial x^{\alpha}}(x,t) = \frac{1}{\Gamma(m-\alpha)}\frac{\partial^m}{\partial x^m}\int_0^{x} u(\xi,t)(x-\xi)^{m-1-\alpha} d\xi. \quad (6)$$

Formally when subjected to the fractional Neumann condition we have the following problem, for $1 < \alpha < 2$,

$$\frac{\partial u}{\partial t}(x,t) = D\frac{\partial^{\alpha}_{0} u}{\partial x^{\alpha}}(x,t), \quad x > 0, \quad (7)$$

$$\frac{\partial^{\alpha-1}_{0} u}{\partial x^{\alpha-1}}(0,t) = 0, \quad (8)$$

with an initial condition $u(x,0) = u_0(x)$, $x \geq 0$.

3 The Numerical Methods

We start to present an implementation for the case when we have an open domain and then show how to adjust it to the presence of both types of boundaries.

3.1 Open Domain

For the problem defined in the whole real line, the domain discretisation is given by $x_j = x_{j-1} + \Delta x,\ j \in \mathbb{Z}$ and the time discretization $t_n = n\Delta t$, $n \geq 0$ integer.

We approximate the left Riemann-Liouville fractional derivative by the well-known Grünwald-Letnikov approximation. Define the Grünwald-Letnikov coefficients, for all $\alpha > 0$, using the following recurrence formula

$$g_0^\alpha = 1, \quad g_{k+1}^\alpha = -\frac{\alpha - k}{k+1} g_k^\alpha, \quad k \geq 0. \tag{9}$$

The Grünwald-Letnikov approximation, at (x_j, t_n), is given by [12]

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x_j, t_n) \approx \frac{1}{(\Delta x)^\alpha} \sum_{k=0}^{\infty} g_k^\alpha u(x_{j-k+1}, t_n). \tag{10}$$

Let U_j^n represent the approximate solution of $u(x_j, t_n)$ in the discrete domain and define

$$\mu_\alpha = \frac{D\Delta t}{(\Delta x)^\alpha}.$$

The Euler explicit method to approximate the fractional diffusion equation will be now given by

$$U_j^{n+1} = U_j^n + \mu_\alpha \sum_{k=0}^{\infty} g_k^\alpha U_{j-k+1}^n, \quad \text{for all} \quad j \in \mathbb{Z}. \tag{11}$$

The matricial form of the numerical method in the open domain takes in consideration that the function goes to zero as we go to infinity and we have $\mathbf{U}^{n+1} = (\mathbf{I} + \mu_\alpha \mathbf{A})\mathbf{U}^n$, with $\mathbf{U}^n = [U_{-N}^n, \ldots, U_N^n]^T$, $\mathbf{I}$ is the identity matrix and the matrix $\mathbf{A}$ is given by

$$\mathbf{A} = \begin{bmatrix} g_1^\alpha & g_0^\alpha & 0 & \ldots & 0 & 0 \\ g_2^\alpha & g_1^\alpha & g_0^\alpha & \ldots & 0 & 0 \\ g_3^\alpha & g_2^\alpha & g_1^\alpha & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ g_{2N+1}^\alpha & g_{2N}^\alpha & g_{2N-1}^\alpha & \cdots & g_2^\alpha & g_1^\alpha \end{bmatrix}.$$

The following result indicates that in the open domain, the approximation (10) is of order one. This result was given for a function that only depends on x, but this can be easily adjusted for the case under discussion.

Theorem 1 [12]**.** *Let $m - 1 < \alpha < m$, $u(\cdot, t) \in C^{[\alpha]+m+1}(\mathbb{R})$, for a fixed t, such that all the derivatives, in x, up to order $[\alpha] + m + 2$ belong to $L^1(\mathbb{R})$ and where $[\alpha]$ represents the integer part of α. Then the fractional Riemann-Liouville derivative given by (1) satisfies*

$$\frac{\partial^\alpha u}{\partial x^\alpha}(x_j, t) = \frac{1}{(\Delta x)^\alpha} \sum_{k=0}^{\infty} g_k^\alpha u(x_j - (k-1)\Delta x, t) + O((\Delta x)).$$

Since we have considered an explicit numerical method, we have a conditionally stable scheme and the stability conditions can be obtained using the von Neumann analysis or Fourier analysis [11].

Theorem 2. *If the numerical method (11) is von Neumann stable then* $\mu_\alpha \leq 2^{1-\alpha}$.

When imposing a boundary the von Neumann stability condition is a necessary condition for the stability of the numerical method with boundaries.

3.2 The Reflective Boundary

The domain discretisation is given by $x_j = x_{j-1} + \Delta x,\ j \in \mathbb{Z}$. When we have a reflecting boundary condition at $x = 0$, since the left fractional derivative is modified to (3), because $U^n_{j-i+1} = U^n_{-j+i-1}$, the approximation becomes

$$\frac{\delta^\alpha_{ref} u(x_j,t)}{(\Delta x)^\alpha} \approx \frac{1}{(\Delta x)^\alpha}\sum_{i=0}^{j+1} g^\alpha_i U^n_{j-i+1} + \frac{1}{(\Delta x)^\alpha}\sum_{i=j+2}^{\infty} g^\alpha_i U^n_{j-i+1}$$
$$= \frac{1}{(\Delta x)^\alpha}\sum_{i=0}^{j+1} g^\alpha_i U^n_{j-i+1} + \frac{1}{(\Delta x)^\alpha}\sum_{i=j+2}^{\infty} g^\alpha_i U^n_{i-j-1}.$$

Consider the explicit Euler scheme to approximate Eq. (4) given by

$$U^{n+1}_j = U^n_j + \mu_\alpha \delta^\alpha_{ref} U^n_j. \tag{12}$$

In this case the matricial form of the problem is $\mathbf{U}^{n+1} = (\mathbf{I} + \mu_\alpha \mathbf{A_{Sym}})\mathbf{U}^n$, with $\mathbf{U}^n = [U^n_0, \ldots, U^n_N]^T$, $\mathbf{I}$ is the identity matrix and the matrix $\mathbf{A_{Sym}}$ is

$$\mathbf{A_{Sym}} = \begin{bmatrix} g^\alpha_1 & g^\alpha_0 + g^\alpha_2 & g^\alpha_3 & \cdots & g^\alpha_{N-2} & g^\alpha_{N-1} \\ g^\alpha_2 & g^\alpha_1 + g^\alpha_3 & g^\alpha_0 + g^\alpha_4 & \cdots & g^\alpha_{N-1} & g^\alpha_N \\ g^\alpha_3 & g^\alpha_2 + g^\alpha_4 & g^\alpha_1 + g^\alpha_5 & \cdots & g^\alpha_N & g^\alpha_{N+1} \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ g^\alpha_{2N+1} & g^\alpha_{2N} + g^\alpha_{N+2} & g^\alpha_{2N-1} + g^\alpha_{N+3} & \cdots & g^\alpha_2 + g^\alpha_{2N} & g^\alpha_1 + g^\alpha_{2N+1} \end{bmatrix}.$$

The changes of the entries of the matrix $\mathbf{A}$ due to the presence of this reflecting boundary are displayed in gray color.

This problem is equivalent to a problem defined in the real line and therefore the stability conditions of the numerical method are similar to those obtained for the open problem.

3.3 The Fractional Boundary

If we are in a bounded domain and consider the approximation (10) directly in that domain, we can arrive at the following approximation in the interior points

$$U^{n+1}_j = U^n_j + \mu_\alpha \sum_{i=0}^{j+1} g^\alpha_i U^n_{j-i+1},\ j = 0, \ldots, N-1. \tag{13}$$

However in this case we can see that no mass has been moved. To enforce the boundary condition, we modify the Euler scheme (13) at the point $x = 0$. Let us see how we can impose the boundary condition (8). We give here a mathematical approach, instead of the physical interpretation given in [2].

Taking in consideration the properties of the Riemann-Liouville fractional derivative the differential Eq. (7) at $x = 0$ can be written as

$$\frac{\partial u}{\partial t}(0,t) = D\frac{\partial}{\partial x}\left(\frac{\partial_0^{\alpha-1} u}{\partial x^{\alpha-1}}\right)(0,t).$$

We can use the Euler approximation for the time derivative, that is,

$$\frac{\partial u}{\partial t}(0,t) \approx \frac{U_0^{n+1} - U_0^n}{\Delta t}.$$

A first order approximation for the first order spatial derivative allow us to write

$$\frac{\partial}{\partial x}\left(\frac{\partial_0^{\alpha-1} u}{\partial x^{\alpha-1}}\right)(0,t) \approx \frac{1}{\Delta x}\left(\frac{\partial_0^{\alpha-1} u}{\partial x^{\alpha-1}}(x_1,t) - \frac{\partial_0^{\alpha-1} u}{\partial x^{\alpha-1}}(0,t)\right). \tag{14}$$

We know the value of the second term on the right hand side of (14), since this is the boundary condition. Additionally, we can approximate the fractional derivative at x_1 using the Grünwald-Letnikov approximation, that is,

$$\frac{\partial_0^{\alpha-1} u}{\partial x^{\alpha-1}}(x_1,t_n) \approx \frac{1}{(\Delta x)^{\alpha-1}}\sum_{k=0}^{1} g_k^{\alpha-1} U_{1-k}^n.$$

Therefore, we obtain

$$U_0^{n+1} = U_0^n + \mu_\alpha(g_1^{\alpha-1}U_0^n + g_0^{\alpha-1}U_1^n).$$

Finally, the numerical method is given by

$$\begin{aligned} U_j^{n+1} &= U_j^n + \mu_\alpha \sum_{i=0}^{j+1} g_{j-i+1}^\alpha U_i^n,\ j = 1,\ldots,N, \\ U_0^{n+1} &= U_0^n + \mu_\alpha(g_1^{\alpha-1}U_0^n + g_0^{\alpha-1}U_1^n). \end{aligned}$$

In this case the matricial form of the problem is $\mathbf{U}^{n+1} = (\mathbf{I} + \mu_\alpha \mathbf{A_{Neu}})\mathbf{U}^n$, with $\mathbf{U}^n = [U_0^n, \ldots, U_N^n]^T$, $\mathbf{I}$ is the identity matrix and the matrix $\mathbf{A_{Neu}}$ is given by

$$\mathbf{A_{Neu}} = \begin{bmatrix} g_1^{\alpha-1} & g_0^{\alpha-1} & 0 & \ldots & 0 & 0 \\ g_2^\alpha & g_1^\alpha & g_0^\alpha & \ldots & 0 & 0 \\ g_3^\alpha & g_2^\alpha & g_1^\alpha & \ldots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ g_{2N+1}^\alpha & g_{2N}^\alpha & g_{2N-1}^\alpha & \cdots & g_2^\alpha & g_1^\alpha \end{bmatrix}.$$

The changes of the entries of the matrix $\mathbf{A}$ due to the presence of this boundary are in the first line and in gray color.

Theorem 3. *If $\mu_\alpha \leq 1/\alpha$ then the eigenvalues of the matrix iteration* $\mathbf{I} + \mu_\alpha \mathbf{A_{Neu}}$ *are less than one.*

The previous result can be proved using the Gersghorin theorem.

The numerical experiments show that the stability region is given by the necessary stability condition $\mu_\alpha \leq 2^{1-\alpha}$ and not by this more restrictive sufficient stability condition $\mu_\alpha \leq 1/\alpha$.

4 The Influence of the Boundaries

We illustrate the effect of the boundaries for different values of α. We consider the approximation of the solution of the fractional diffusion equation with an initial condition that is an approximation of the Dirac delta function, that is,

$$u_0(x) = \frac{1}{\epsilon\sqrt{\pi}} \mathrm{e}^{-(x-x_0)^2/\epsilon^2},$$

for a small $\epsilon > 0$. For all figures we have taken $D = 1$, $\epsilon = 0.1$, $x_0 = 1$.

In the next figures we consider two values of α, that is, $\alpha = 1.3$ in Fig. 1 and $\alpha = 1.8$ in Fig. 2. As we evolve in time, the effect of the boundaries on the solution is quite relevant. By the figures we can also see that in the open domain we have an asymmetric case since we are only considering the left Riemann Liouville fractional derivative and therefore the wave has a significant heavy tail on the right hand side, when α is closer to 1.

Near the boundary, the behaviour of the solution with the Neumann boundary can be unexpected at first. However, the steady state general solution of the fractional diffusion Eq. (2) is the combination of the functions $x^{\alpha-1}$ and $x^{\alpha-2}$. The solution that goes to zero as x goes to infinity is $x^{\alpha-2}$. This is also the function that better describes the behaviour we observe in the previous figures, near the boundary, that is, the solution $x^{\alpha-2}$ goes to infinity as x goes to zero.

We have seen the consequences of having two types of reflecting boundaries. Near the boundary the solutions behave very differently, highlighting that they

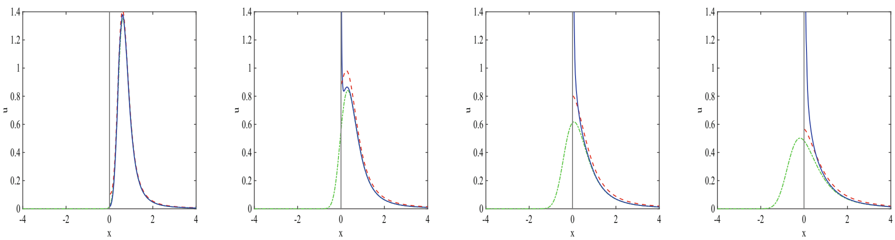

Fig. 1. Plots of $u(x,t)$ for $x_0 = 1$, $D = 1$, $\alpha = 1.3$. Open domain in green line $(- \cdot -)$; Symmetric boundary in red line $(--)$; Neumann boundary in blue line $(-)$. Evolution in time described from left to right: $t = 0.25, 0.5, 0.75, 1$.

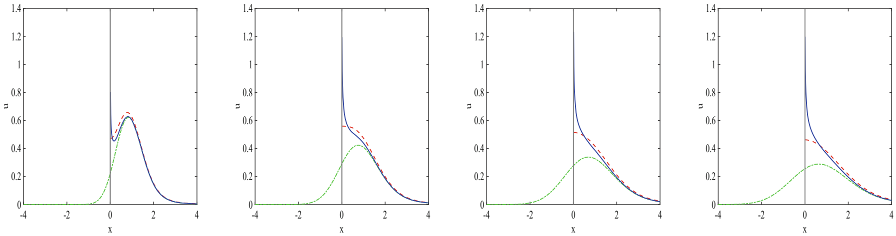

Fig. 2. Plots of $u(x,t)$ for $x_0 = 1$, $D = 1$, $\alpha = 1.8$. Open domain in green line $(- \cdot -)$; Symmetric boundary in red line $(--)$; Neumann Boundary in blue line $(-)$. Evolution in time. Left to right $t = 0.25, 0.5, 0.75, 1$.

represent completely different physical phenomena. Far away from the boundary the behaviour is similar in all three cases: open domain, symmetric reflecting boundary and the fractional Neumann boundary.

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