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On reflecting boundary conditions for space-fractional equations on a finite interval: Proof of the matrix transfer technique

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ABSTRACT

Even in the one-dimensional case, dealing with the analysis of space-fractional differential equations on finite domains is a difficult issue. On a finite interval coupled with zero flux boundary conditions, different approaches have been proposed to define a space-fractional differential operator and to compute the solution to the corresponding fractional problem, but to the best of our knowledge, a clear relationship between these strategies is yet to be established. Here, by using the theory of α-stable symmetric Lévy flights and the master equation, we derive a discrete representation of the non-local operator embedding in its definition the concept of reflecting boundary conditions. We refer to this discrete operator as the reflection matrix and provide (and prove) a theorem on the analytic expression of its eigenvalues and eigenvectors. We then use this result to compare the reflection matrix to the discrete operator defined via the matrix transfer technique, and establish the validity of the latter technique in producing the correct solution to a space-fractional differential equation on a finite interval with reflecting boundary conditions. We finally discuss and emphasize the challenges in the generalisation of the proposed result to more than one spatial dimension.

1. Introduction

The use of fractional differential equations to model anomalous transport phenomena [1] involving diffusion processes whose characteristics substantially deviate from the classical Gaussian and Markovian assumptions, is a field of rapidly growing interest with applications in many different fields. These include the study of rotating flows [2], disordered media [3], hydrology [4], fluid dynamics in porous media [5–7], biology [8,9], medicine [10], neural [11] and cardiac electrophysiology [12]. Fractional models are typically obtained by substituting the classical differential operators in space or time (or both) with a non-integer counterpart. The link between fractional diffusion and anomalous transport can be clearly understood with the theory of random walks [13]. In the context of space-fractional models, the fractional Laplacian $(-\Delta)^{\alpha/2}$ [14] plays a fundamental role due to its probabilistic interpretation. In fact, for $\alpha \in (0, 2]$, the space-fractional diffusion

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equation

$$\partial_t u = -\mathcal{K}_\alpha(-\Delta)^{\alpha/2} u, \tag{1}$$

where $\mathcal{K}_\alpha$ is a suitable scaling coefficient, can be interpreted as the evolution equation for the probability density function $u(x, t)$ of an ensemble of particles performing a particular type of Continuous Time Random Walk (CTRW) in $\mathbb{R}^n$, known as an α-stable symmetric Lévy flight and characterised by algebraically decaying (non-Gaussian) probability distribution functions of the particle jumps [15].

However, in many practical applications, transport processes occur in finite domains. This leads to two major challenges from the mathematical point of view: the restriction of the operator definition to a finite domain $\Omega \subset \mathbb{R}^n$ and the need of incorporating in the problem formulation a suitable representation of the boundary conditions. In fact, due to the non-locality of the differential operator considered, the mere specification of a local condition for the solution at the boundary (such as a Neumann boundary condition) is no longer sufficient to obtain a well-posed formulation.

The exception is in the case of zero Dirichlet boundary conditions where the solution to the fractional differential equation can be extended so that it is equal to zero on the complement of the bounded domain (see, for example, Wang and Basu [16] for a fast finite-difference algorithm for space-fractional diffusion equations with these boundary conditions).

The treatment of all other types of boundary conditions is not at all straightforward and a unified theory determining a common approach to the solution of all these non-trivial cases is still missing, even for one spatial dimension. In line with the work by Zoia et al. [17], we are interested in describing how Lévy flights are affected by the introduction of a particular type of boundary conditions and in showing how the spectrum of the nonlocal operator governing the corresponding fractional differential equation change when restricting the spatial domain to a finite interval. As in the papers by Chen et al. [18], Defterli et al. [19], and D'Elia and Gunzburger [20], we focus on symmetric processes and symmetric fractional derivatives, leaving the analysis of the non-symmetric framework as future extension of this work. In particular, in this paper we analyse the case of homogeneous Neumann boundary conditions (also referred to as zero flux or insulating boundary conditions) for a one-dimensional finite domain $[0, L]$ with $L > 0$, and establish an important connection between the following two existing approaches that to the best of our knowledge has not appeared in the literature.

On one hand, we consider the practical approach originally proposed by Ilić et al. [21,22], known as the Matrix Transfer Technique (MTT). This method consists in defining a discrete representation of the fractional Laplacian on a bounded domain by raising to a fractional power α the classical discrete Laplacian coupled to a given set of standard boundary conditions. This fractional power is computed via a diagonalisation of the standard operator. Let B be the discrete Laplacian coupled to standard homogeneous Neumann boundary conditions and let $B = VDV^{-1}$ be a diagonalisation of B (with D diagonal matrix of eigenvalues and the columns of V being eigenvectors of B). Then, the discrete fractional operator $B^{\alpha/2}$ defined via the MTT is given by $B^{\alpha/2} = VD^{\alpha/2}V^{-1}$, where $D^{\alpha/2}$ is the diagonal matrix of the fractional powers of the eigenvalues of B. Although, this approach provides a convenient practical tool for the computation of the solution to a given space-fractional problem via the method of lines, there is no proof that by raising the standard operator to a fractional power, the resulting matrix carries the correct representation of the boundary conditions for the non-local problem restricted to the finite domain.

On the other hand, Krepysheva et al. [23] and Néel et al. [24] use the Generalised Master Equation (GME) [25] and the theory of α-stable symmetric Lévy flights to derive a space-fractional equation involving a restriction of the unbounded fractional Laplacian to a semi-infinite interval and a finite interval, respectively. This theoretical approach is essentially based on the method of images [26] and the idea of interpreting an insulating boundary condition as a reflecting wall for the trajectories of the particles performing the considered CTRW. In this case, although the authors of [23] and [24] derive fractional operators embedding in their definition the concept of reflecting boundary conditions and hence the correct representation of insulating boundaries, an explicit strategy describing how to use this theoretical formulation in order to compute the solution of the considered space-fractional problem is missing.

In this paper, we bring together these ideas and prove that in one spatial dimension the MTT, where the standard operator is coupled with homogeneous Neumann boundary conditions, is indeed correct and leads to the proper representation of reflecting boundaries for the fractional case.

In Section 2, we review the theoretical approach of [23] and [24], and reformulate the main results therein by introducing a convenient sawtooth function representation. This reformulation, together with a natural modification of the shifted Grünwald–Letnikov finite-difference scheme [27], allows us in Section 3 to obtain a discrete representation of the nonlocal operator with the modified kernel accounting for the two reflecting boundary conditions on the bounded domain, which we refer to as the reflection matrix. We then address our fundamental question concerning the relationship between the fractional operator embedding reflecting boundary conditions and the spectral definition of the fractional Laplacian on which the MTT is based. In particular, in Section 4.2 we prove the convergence of the spectra of both discrete operators towards the same limit (as the number of nodes in the spatial discretisation of the finite interval goes to infinity) and we validate the use of a spectral technique as efficient solution strategy for the space-fractional problem. Furthermore, we make some additional remarks on how the concept of fractional flux can be interpreted and computed at the end points of the considered finite domain in presence of two reflecting boundary conditions. Our final conclusions and a discussion about extensions of this result to more than one spatial dimension and regular or irregular bounded domains are given in Section 5.

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