

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

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one spatial dimension.

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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], [6], [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 equation

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

where \mathcal{K}_α 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

25 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
 30 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 straight-
 35 forward 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
 40 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 anal-
 45 yse 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.

50 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
 55 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 $B^{\alpha/2} = VD^{\alpha/2}V^{-1}$,
60 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
65 conditions for the non-local problem restricted to the finite domain.

On the other hand, Krepyshcheva 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,
70 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
75 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
80 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
85 shifted Grünwald–Letnikov finite-difference scheme [27], allows us in Section 3 to obtain a discrete representation of the non-local 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.

2. Lévy flights on the insulated interval $[0, L]$

Let us consider an ensemble of particles performing an α -stable symmetric Lévy flight on the unbounded domain \mathbb{R} . Let T_i be the independent identically distributed (iid) positive random variables representing the waiting times between consecutive particle jumps, and X_i be the iid (not necessarily positive) random variables representing the jump lengths. In this CTRW, the X_i and the T_i are independent, that is, the jump length probability density function (pdf) and the waiting time pdf are decoupled. If $\Lambda_l(x, x')dx$ denotes the probability that a particle jumps from x' and arrives in $[x, x + dx]$, also known as the transition probability, then, in the unbounded domain, the probability $P(x, t)dx$ of finding a particle in $[x, x + dx]$ at an instant t satisfies the GME given by

$$P(x, t) = \delta_{x_0}(x) \int_{t'=t}^{\infty} \psi_{\tau_0}(t') dt' + \int_{\mathbb{R}} \int_{t'=0}^t P(x', t') \Lambda_l(x, x') \psi_{\tau_0}(t - t') dt' dx', \quad (2)$$

where $\psi_{\tau_0}(t) := e^{-t/\tau_0}/\tau_0$ is the Markovian pdf of T_i , τ_0 can be viewed as the characteristic time scale of the waiting times, x_0 is the initial starting position of the particle and $\delta_{x_0}(x)$ is the Dirac delta function. In the absence of nonuniform
115 force fields, a random variable X exists, such that the X_i are distributed as lX [23]. Furthermore, as highlighted by Krepyshcheva et al. [23], the parameter l can be thought of as being the length scale of the microscopic motion. Assuming that the pdf $\phi_1(\cdot)$ of the random variable X is a symmetric α -stable Lévy law $p_\alpha(\cdot, 0)$ of order $\alpha \in (0, 2]$, whose characteristic function is $e^{-|k|^\alpha}$ [28], the
120 resulting transition pdf between locations x' and x is $\Lambda_l(x, x') = \phi_l(x - x')$ with $\phi_l(X) = \phi_1(X/l)/l$ and $\phi_1(X) = p_\alpha(X, 0)$.

If we consider a force field constraining the particles to never leave the finite domain $[0, L]$, we introduce insulating (zero-flux) boundary conditions for our spatial domain. Under these assumptions given an initial position $x_0 \in [0, L]$, we
125 obtain a modified GME for $P(x, t)$ that involves an integral over $[0, L]$ instead of \mathbb{R} , and equation (2) becomes

$$P(x, t) = \delta_{x_0}(x) \int_{t'=t}^{\infty} \psi_{\tau_0}(t') dt' + \int_{x'=0}^L \int_{t'=0}^t P(x', t') \Lambda_l^L(x, x') \psi_{\tau_0}(t - t') dt' dx', \quad (3)$$

where $\Lambda_l^L(x, x')$ is a modified transition probability. In the GME (3), x and x' are both bound to the finite domain $[0, L]$. Our aim is to obtain a suitable definition of $\Lambda_l^L(x, x')$ and to derive a macroscopic transport equation for P on
130 this finite domain.

Insulating boundaries are viewed as reflecting walls affecting the parabolic trajectory of particles jumping in (x, z) coordinates in a uniform force field (with direction z orthogonal to x). When a bouncing particle hits the reflecting barrier, the assumption of no energy exchange with the wall results in a
135 change of sign of the x component of the momentum so that the trajectory simply follows the mirror image of the portion of parabola located outside of the domain. Hence, the presence of the reflecting condition, can be interpreted mathematically as the introduction of a symmetric correspondence of points lo-

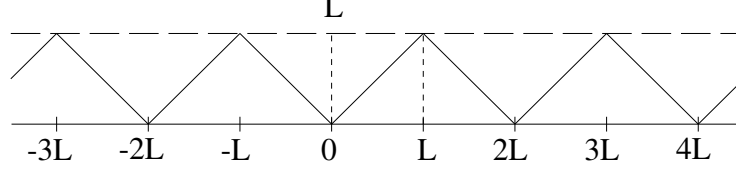


Figure 1: The continuous sawtooth function $[x]_0^L$.

cated at the same distance from the wall but on different sides of it. When two
140 reflecting boundaries are considered, the case of multiple bounces between the
walls becomes possible and a jump from x' to x , with both $x', x \in [0, L]$, can be
obtained in an infinite number of ways.

A simple way to represent the combination of the two symmetry conditions
introduced by the two reflecting boundaries and the resulting identification of
145 points of the unbounded domain with their corresponding $x \in [0, L]$ under
reflections is given by the sawtooth function graphically represented in Figure 1
and denoted by $[\cdot]_0^L$. This function coincides with the absolute value in the
interval $[-L, L]$ and is then extended periodically with period $2L$ to the entire
unbounded domain (so that it preserves symmetry about both $x = 0$ and $x = L$).

In order to define $\Lambda_l^L(x, x')$, for a fixed $x \in [0, L]$, we let S_x represent the set
150 $S_x := \{y \in \mathbb{R} \mid [y]_0^L = x\}$, that is, the set of points in the unbounded domain
that can be identified with $x \in [0, L]$ under repeated reflections between the two
boundaries. Due to the symmetry and the periodicity of the sawtooth function,
for a fixed $x \in [0, L]$, we obtain $S_x = \{x + 2mL, -x + 2mL \mid m \in \mathbb{Z}\}$. Hence,
155 for $x, x' \in [0, L]$, the transition probability $\Lambda_l^L(x, x')$ of equation (3) can be
expressed as

$$\Lambda_l^L(x, x') = \sum_{y \in S_x} \phi_l(y - x') = \sum_{m \in \mathbb{Z}} \phi_l(\pm x + 2mL - x').$$

Let $P_\infty(x, t) := P([x]_0^L, t)$ for all $x \in \mathbb{R}$, that is, let P_∞ be the periodic
extension of P with period $2L$, defined such that $P_\infty = P$ on $[0, L]$ and P_∞ is

symmetric with respect to both ends of $[0, L]$. From equation (3) we find that

160 P_∞ satisfies the following GME on \mathbb{R} :

$$P_\infty(x, t) = g_0(x) \int_{t'=t}^{\infty} \psi_{\tau_0}(t') dt' + \int_{\mathbb{R}} \int_{t'=0}^t P_\infty(x', t') \phi_l(x - x') \psi_{\tau_0}(t - t') dt' dx', \quad (4)$$

where $g_0(x) := \sum_{m \in \mathbb{Z}} [\delta_{x_0+2mL}(x) + \delta_{-x_0+2mL}(x)]$ is the sum of two shifted Dirac combs and corresponds to the initial condition $\delta_{x_0}(x)$ for P .

By using the theory of Fourier–Laplace transforms (see Appendix A) we can then show that P_∞ is the solution on \mathbb{R} of the fractional diffusion equation

$$\begin{cases} \partial_t P_\infty(x, t) = -K_\alpha (-\Delta)^{\alpha/2} P_\infty(x, t) \\ P_\infty(x, 0) = g_0(x), \end{cases} \quad (5)$$

165 where K_α is the constant ratio $K_\alpha := l^\alpha / \tau_0$.

We now use the relationship between P and P_∞ to obtain a suitable transport equation for P on $[0, L]$. As proved by Yang [29], in the unbounded one-dimensional case, $-(-\Delta)^{\alpha/2} = \mathcal{R}_x^\alpha$, where \mathcal{R}_x^α is the Riesz–Feller operator defined as follows [28]:

$$\mathcal{R}_x^\alpha := -[c_\alpha I_+^{-\alpha} + c_\alpha I_-^{-\alpha}], \quad (6)$$

170 with $c_\alpha := \frac{1}{2 \cos(\pi\alpha/2)}$ and for a sufficiently well-behaved function $f(x)$ and $\alpha \in (1, 2)$,

$$I_+^{-\alpha} f(x) := \frac{1}{\Gamma(2-\alpha)} \partial_x^2 \int_{-\infty}^x (x-y)^{1-\alpha} f(y) dy, \quad (7)$$

$$I_-^{-\alpha} f(x) := \frac{1}{\Gamma(2-\alpha)} \partial_x^2 \int_x^{\infty} (y-x)^{1-\alpha} f(y) dy. \quad (8)$$

Therefore, P_∞ satisfies

$$\begin{aligned} \partial_t P_\infty(x, t) &= K_\alpha \mathcal{R}_x^\alpha P_\infty(x, t) \\ &= K_\alpha \frac{-c_\alpha}{\Gamma(2-\alpha)} \partial_x^2 \int_{\mathbb{R}} |x-y|^{1-\alpha} P_\infty(y, t) dy. \end{aligned} \quad (9)$$

Let $\mathcal{R}_{x,L}^\alpha$ be the non-local operator with modified kernel embedding the
175 effect of two reflecting boundary conditions, that is, the operator such that for a sufficiently well-behaved $f(x)$ defined on $[0, L]$,

$$\mathcal{R}_{x,L}^\alpha f(x) := \frac{-c_\alpha}{\Gamma(2-\alpha)} \partial_x^2 \int_{\mathbb{R}} |x-y|^{1-\alpha} f([y]_0^L) dy. \quad (10)$$

From the definition of P_∞ and equation (9) we hence conclude that, for $t > 0$, P is the solution of the fractional transport equation

$$\partial_t P(x, t) = K_\alpha \mathcal{R}_{x,L}^\alpha P(x, t),$$

on the insulated domain $[0, L]$, with initial condition $P(x, 0) = \delta_{x_0}(x)$ and operator $\mathcal{R}_{x,L}^\alpha$ given by (10).
180

We stress that in deriving the operator $\mathcal{R}_{x,L}^\alpha$ embedding in its definition the concept of insulating boundaries, we simply use the GME and do not impose any additional nonlocal condition at the finite ends of the spatial domain as is the case in the work by Baeumer et al. [30] for the fractional flux at the boundary
185 $x = 0$ of the semi-infinite interval $[0, \infty)$. This quantity is indeed not clearly defined on a bounded domain with non-trivial boundary conditions and hence a suitable modification or different interpretation should be given to the concept of fractional flux in the presence of two reflecting boundaries (see Section 3.1 for some additional considerations on this).

190 3. Construction of the reflection matrix

In this section, we develop a discrete approximation of $\mathcal{R}_{x,L}^\alpha f(x)$ for a function f defined on the insulated interval $[0, L]$, by adapting the shifted Grünwald–Letnikov approach proposed by Meerschaert and Tadjeran [27], for the approximation of \mathcal{R}_x^α in the unbounded case.

From definition (10), we see that the operator $\mathcal{R}_{x,L}^\alpha$ can be rewritten as the following sum:

$$\mathcal{R}_{x,L}^\alpha = -[c_\alpha S_+ + c_\alpha S_-],$$

195 where, again, $c_\alpha = \frac{1}{2 \cos \pi \alpha / 2}$, and given f on $[0, L]$ we define

$$S_+ f(x) := \frac{1}{\Gamma(2-\alpha)} \partial_x^2 \int_{-\infty}^x (x-y)^{1-\alpha} f([y]_0^L) dy,$$

$$S_- f(x) := \frac{1}{\Gamma(2-\alpha)} \partial_x^2 \int_x^\infty (y-x)^{1-\alpha} f([y]_0^L) dy.$$

The integrals in the expression of S_+ and S_- can be viewed (up to a constant) as Weyl integrals of the function $\bar{f} := f([y]_0^L)$ which is defined on \mathbb{R} and periodic with period $2L$. For these integrals to be well defined, we assume that $f \in C([0, L])$ and that the integral of \bar{f} over its period is equal to zero. For a more detailed analysis on the existence and uniqueness of the solution to the considered fractional problem under the above hypothesis we refer the reader to the work by Szekeres and Izsák [31]. On the unbounded domain, the approximation of \mathcal{R}_x^α is based on the definition of two shifted Grünwald–Letnikov operators approximating the pseudo-differential operators I_+ and I_- given by equations (7) and (8), respectively. Similarly, given a small step length h , we define here two modified shifted Grünwald–Letnikov operators¹, ${}_hS_+$ and ${}_hS_-$, for the approximation of S_+ and S_- , respectively:

$${}_hS_+f(x) := \frac{1}{h^\alpha} \sum_{j=0}^{\infty} \omega_j f([x - (j-1)h]_0^L),$$

$${}_hS_-f(x) := \frac{1}{h^\alpha} \sum_{j=0}^{\infty} \omega_j f([x + (j-1)h]_0^L),$$

where $(\omega_j)_0^\infty$ is the sequence of weights of the classical Grünwald–Letnikov strategy, defined as $\omega_j := (-1)^j \binom{\alpha}{j}$, for all $j \geq 0$.

To obtain the modified finite-difference scheme approximating the operator $\mathcal{R}_{x,L}^\alpha$, let us consider a spatial discretisation of the finite domain $[0, L]$ by introducing a uniform mesh of $N + 1$ nodes $x_i = ih$, with mesh size $h = \frac{L}{N}$, and $i = 0, 1, \dots, N$. Let $f_i \approx f(x_i)$. By using the definitions of ${}_hS_+$ and ${}_hS_-$, for $i = 0, 1, \dots, N$, at each node x_i we obtain the following approximation of $\mathcal{R}_{x,L}^\alpha f$:

$$\mathcal{R}_{x,L}^\alpha f \Big|_{x=x_i} \approx \frac{-c_\alpha}{h^\alpha} \sum_{j=0}^{\infty} \omega_j \left(f_{[i-j+1]_0^N} + f_{[i+j-1]_0^N} \right), \quad (11)$$

¹The modified approach proposed here is actually equivalent to applying the classical shifted Grünwald–Letnikov scheme to the periodic (with period $2L$) and even extension of the given function f defined on $[0, L]$. Therefore, as in the classical case, the proposed approximation is still first order accurate in space.

where $[\cdot]_0^N$ denotes the discrete version of the continuous sawtooth function $[\cdot]_0^L$, that is, the restriction of the continuous sawtooth function $[x]_0^L$ to integer values of the argument x . From equation (11), we see that the value of $\mathcal{R}_{x,L}^\alpha f$ at a given node of the spatial mesh is approximated in terms of the solution approximation
220 at all the nodes of the interval discretisation, in agreement with the non-local nature of the operator. Moreover, we observe that for a fixed $i \in \{0, 1, \dots, N\}$, the infinite sum on the right-hand side of equation (11) can be rewritten as

$$\sum_{j=0}^{\infty} \omega_j \left(f_{[i-j+1]_0^N} + f_{[i+j-1]_0^N} \right) = \sum_{k=0}^N M_{i,k} f_k, \quad (12)$$

where each $M_{i,k}$ is an infinite sum of weights ω_j with indices chosen in suitable subsets $W_{i,k} \subset \mathbb{Z}_0^+$ (where \mathbb{Z}_0^+ denotes the set of all non-negative integers). In
225 particular, given $i, k \in \{0, 1, \dots, N\}$,

$$M_{i,k} = \sum_{j \in W_{i,k}} \omega_j, \quad \text{with } W_{i,k} := \{j \in \mathbb{Z}_0^+ \mid [i+j-1]_0^N = k \text{ or } [i-j+1]_0^N = k\}.$$

By using the definition of $[\cdot]_0^N$, we notice that $[i+j-1]_0^N = k$ if and only if $j = \pm k - i + 1 + 2mN$ for some integer m , and $[i-j+1]_0^N = k$ if and only if $j = \pm k + i + 1 + 2mN$ for some integer m . Therefore, the $M_{i,k}$ can be rewritten as suitable sums of subseries of the form

$$\sum_{m \in \mathbb{Z}_0^+} \omega_{2mN+r} \quad \text{for some } r \in \{0, 1, 2, \dots, 2N-1\}. \quad (13)$$

230 Let \mathbf{f} denote the vector of $N+1$ approximations of $f(x)$ at the $N+1$ nodes of the spatial mesh for $[0, L]$. Combining equation (11) and equation (12) for all values of $i \in \{0, 1, \dots, N\}$, we find that $\mathcal{R}_{x,L}^\alpha f$ can be approximated by a matrix vector product as $\mathcal{R}_{x,L}^\alpha f \approx -A_{\alpha,h} \mathbf{f}$, where $A_{\alpha,h} := \frac{c_\alpha}{h^\alpha} M$, h is the uniform mesh size, c_α the usual trigonometric coefficient, and M is the square matrix of size
235 $N+1$ with entries $M_{i,k}$ defined above ($i, k \in \{0, 1, \dots, N\}$).

The reflection matrix $A_{\alpha,h}$ is diagonally dominant and its sign has been chosen so that its diagonal entries are always non-negative. Moreover, in the particular case $\alpha = 2$, $c_\alpha = -1/2$ and the only non-zero weights in the sequence $(\omega_j)_0^\infty$ are $\omega_0 = 1$, $\omega_1 = -2$ and $\omega_2 = 1$. As a result, $A_{2,h}$ is equal to the discrete

240 Laplacian on $[0, L]$ coupled with homogeneous Neumann boundary conditions, obtained with a finite-difference approximation on a uniform mesh of $N + 1$ nodes with spacing $h = \frac{L}{N}$ and with a second order approximation of the first order derivative at both ends of $[0, L]$:

$$A_{2,h} = \frac{1}{h^2} \begin{bmatrix} 2 & -2 & & & \\ -1 & 2 & -1 & & \\ & \ddots & \ddots & \ddots & \\ & & -1 & 2 & -1 \\ & & & -2 & 2 \end{bmatrix}. \quad (14)$$

Note that, despite the non-symmetric form of the real tridiagonal matrix in
 245 equation (14), the sign of its entries is symmetric and hence the products of
 corresponding off-diagonal elements ($a_{i+1,i}$ and $a_{i,i+1}$) are strictly positive for
 all $i = 1, \dots, N$. Due to this property, via a suitable change of basis, the consid-
 ered tridiagonal matrix can be shown to be similar to a real symmetric matrix.
 Therefore, its eigenvalues are guaranteed to be real and a diagonalisation of the
 250 tridiagonal matrix exists.

3.1. Some considerations on fractional flux

The nonlocal operator considered in our work and embedding in its definition
 the concept of reflecting boundary conditions was obtained without imposing
 any local condition on the left/right fractional flux at the boundaries of the
 255 spatial interval $[0, L]$. The right fractional flux at $x = 0$, denoted by $D_{-x}^{\alpha-1}$
 according to the notation used by Baeumer et al. in [30], is not clearly defined
 in the presence of a second reflecting boundary at $x = L$. However, by using
 the sawtooth function previously introduced we can modify the definition of the
 operator of fractional order $\alpha - 1$ as follows

$$D_{-x}^{\alpha-1} u(x) := \lim_{h \rightarrow 0^+} \frac{1}{h^{\alpha-1}} \sum_{j=0}^{\infty} \omega_j^{(\alpha-1)} u([x + jh]_0^L), \quad (15)$$

260 where $\omega_j^{(\alpha-1)} = (-1)^j \binom{\alpha-1}{j}$, $\forall j$. Hence, the value of this operator at $x = 0$ can be approximated for a sufficiently small h by

$$D_{-x}^{\alpha-1} u(x) \approx \frac{1}{h^{\alpha-1}} \sum_{j=0}^{\infty} \omega_j^{(\alpha-1)} u_{[j]_0^N}, \quad (16)$$

where $N + 1$ is the number of discretisation nodes used for the spatial interval $[0, L]$, $h = L/N$, and $[\cdot]_0^N$ is the discrete version of our sawtooth function.

The sum in (16) can be rewritten as $\sum_{k=0}^N M_{0,k} u_k$, where

$$M_{0,k} = \sum_{j \in W_{0,k}} \omega_j^{(\alpha-1)} \quad \text{and} \quad W_{0,k} = \{j \in \mathbb{Z}_0^+ \mid [j]_0^N = k\}. \quad (17)$$

265 Letting $g_r = \sum_{m \in \mathbb{Z}_0^+} \omega_{2mN+r}^{(\alpha-1)}$ for $r \in \{0, 1, 2, \dots, 2N-1\}$ we find

$$\sum_{k=0}^N M_{0,k} u_k = g_0 u_0 + \dots + (g_r + g_{2N-r}) u_r + \dots + g_N u_N. \quad (18)$$

In the following section we will use the above expression to make some important considerations on the behaviour of $\frac{1}{h^{\alpha-1}} \sum_{k=0}^N M_{0,k} u_k$ for $N \rightarrow \infty$. Note that the same type of definition, approximation, and considerations can be made for the left fractional flux ($D_{+x}^{\alpha-1}$ in the notation of [30]) at the other end of the
 270 finite interval, $x = L$. Therefore, without loss of generalisation we will only study the case $D_{-x}^{\alpha-1} u(x)$.

4. Results

We begin this section by providing a key result on the analytic expression of the eigenvalues and the eigenvectors of the reflection matrix $A_{\alpha,h}$ for $\alpha \in (1, 2]$.

275 **Theorem 1. [*Eigenvalues and eigenvectors of the reflection matrix*]**
 Let $A_{\alpha,h}$ be the square reflection matrix of order $N + 1$ obtained with the modified shifted Grünwald–Letnikov approach in the approximation of $\mathcal{R}_{x,L}^\alpha$ on the insulated interval $[0, L]$, and let $h = \frac{L}{N}$. Then, for $j = 0, 1, \dots, N$, the j -th eigenvalue μ_j of $A_{\alpha,h}$ can be written as

$$\mu_j = \left[\frac{2}{h} \sin \left(\frac{j\pi}{2N} \right) \right]^\alpha \frac{1}{\cos \left(\frac{\alpha\pi}{2} \right)} \cos \left(\frac{2j + \alpha(N-j)}{2N} \pi \right). \quad (19)$$

280 Moreover, the corresponding $N+1$ eigenvectors φ_j can be described in terms of their components $\varphi_j^{(i)}$ as follows:

$$\varphi_j^{(i)} = \varphi_j^{(0)} \cos\left(\frac{ji\pi}{N}\right), \quad \text{for } i = 0, 1, \dots, N, \quad (20)$$

where $\varphi_j^{(0)}$ is a normalisation constant given by

$$\varphi_j^{(0)} = \begin{cases} \frac{1}{\sqrt{N+1}} & \text{if } j = 0 \text{ or } j = N, \\ \sqrt{\frac{2}{N+2}} & \text{if } j = 1, 2, \dots, N-1. \end{cases} \quad (21)$$

The proof of Theorem 1 is rather lengthy. In order to not disrupt the discussion, we describe here only the general strategy used to obtain the above
285 result and refer the reader to the Supplementary Material for a detailed proof of Theorem 1.

Let $A_{\alpha,h}^{(i)}$ denote the $(i+1)$ -th row of the reflection matrix and $\varphi_j^{(i)}$ the $(i+1)$ -th component of the eigenvector φ_j . For all $j \in \{0, 1, \dots, N\}$, we prove that μ_j, φ_j is an eigenpair of the matrix $A_{\alpha,h}$ by showing that the inner product of
290 $A_{\alpha,h}^{(i)}$ and φ_j is equal to $\mu_j \varphi_j^{(i)}$ for all $i \in \{0, 1, \dots, N\}$. From the considerations made in Section 3, we are able to define analytically each entry of the reflection matrix as the product of the coefficient $\frac{c_\alpha}{h^\alpha}$ and the sum of suitable subseries of the sequence of weights $(\omega_j)_0^\infty$. A fundamental result on the summation of subseries in closed form provided by Chen [32] is the key element of our proof
295 and allows us to rewrite the entries of a given row of the reflection matrix as finite sums of products of complex numbers in trigonometric form. A number of well-established properties of trigonometric functions and a generalisation of De Moivre's formula for powers of complex numbers with exponent α , are then used to rearrange and simplify (via cancellation) the analytic expression of the
300 inner product $A_{\alpha,h}^{(i)} \varphi_j$. An important role in the proof is played by Lagrange's trigonometric identity for the cosine function (e.g., see Jeffrey and Dai [33]). In order to obtain the final equivalence between $A_{\alpha,h}^{(i)} \varphi_j$ and $\mu_j \varphi_j^{(i)}$, different simplification strategies are used depending on the particular combination of indices i, j considered and the odd/even character of the dimension $N+1$.

305 4.1. Comparison with the MTT

From expression (19), we see that each eigenvalue μ_j can be thought of as the product $\lambda_j^{\alpha/2} q_j(\alpha)$ where

$$\lambda_j := \frac{4}{h^2} \sin^2 \left(\frac{j\pi}{2N} \right), \quad (22)$$

and $q_j(\alpha)$ is the term

$$q_j(\alpha) := \frac{1}{\cos\left(\frac{\alpha\pi}{2}\right)} \cos\left(\frac{2j + \alpha(N-j)}{2N}\pi\right). \quad (23)$$

Note that $q_j(2) = 1$ for all j . However, when $\alpha \in (1, 2)$, $q_j(\alpha) = 1$ only for
 310 $j = 0$, while for all other values of $j \in \{1, 2, \dots, N\}$, $q_j(\alpha) \neq 1$.

Let B be the matrix representation of the discrete Laplacian on $[0, L]$, with standard homogeneous Neumann boundary conditions, obtained via the finite-difference approach on the same spatial grid used in the definition of $A_{\alpha,h}$. If a second order approximation for the first order derivative is used at both
 315 boundary nodes, then $B = VDV^{-1}$ where $D = \text{diag}(\lambda_0, \lambda_1, \dots, \lambda_N)$ and $V = [\varphi_0 | \varphi_1 | \dots | \varphi_N]$, with all λ_j given as in equation (22) and the column vectors φ_j as in Theorem 1. Let $B_{\alpha,h}$ denote the fractional operator defined via the MTT as the fractional power of B , that is, $B_{\alpha,h} := VD^{\alpha/2}V^{-1}$. Then, by definition both operators $A_{\alpha,h}$ and $B_{\alpha,h}$ have the same set of eigenvectors and
 320 these vectors are all independent from $\alpha \in (1, 2]$.

Moreover, when $\alpha = 2$, the eigenvalues of $A_{\alpha,h}$ reduce to $\lambda_j, \forall j$, and hence $A_{2,h} = B_{2,h}$. However, in the purely fractional case $\alpha < 2$, the eigenvalues of $A_{\alpha,h}$ and $B_{\alpha,h}$ are distinct and the difference between the spectra of the two operators can be explicitly quantified as the term $q_j(\alpha)$ defined in equation (23)
 325 and non unitary for all $j \in \{1, \dots, N\}$.

4.2. The spectral approach

The above mentioned discrete operators are based on a spatial discretisation of the interval $[0, L]$ involving a finite number $N + 1$ of mesh points. However, it is interesting to study what happens in the limit $N \rightarrow \infty$, and how the increasing
 330 number of nodes affects the discrepancy between the two discrete operators.

Theorem 2. Let $\alpha \in (1, 2]$, $[0, L]$ be a fixed insulated finite domain, and $h = \frac{L}{N}$ the uniform mesh size used to discretise the interval. Then, as h goes to zero, the spectra of the reflecting matrix $A_{\alpha,h}$ and the MTT operator $B_{\alpha,h}$ converge to the same limit, namely the set $\left\{\left(\frac{j\pi}{L}\right)^\alpha\right\}_{j=0}^\infty$.

335 *Proof.* The result simply follows from the fact that for a given fractional index $\alpha \in (1, 2]$, as the number of discretisation nodes approaches infinity (i.e., as $h \rightarrow 0$),

$$\lambda_j \rightarrow \left(\frac{j\pi}{L}\right)^2 \text{ and } q_j(\alpha) \rightarrow 1 \text{ for all } j.$$

Therefore, for the j -th eigenvalue of $A_{\alpha,h}$ and $B_{\alpha,h}$ we find

$$\lim_{N \rightarrow \infty} \mu_j = \lim_{N \rightarrow \infty} \lambda_j^{\alpha/2} = \left(\frac{j\pi}{L}\right)^\alpha. \quad (24)$$

□

340 In light of the above result, we make the following remarks.

Remark 1. Theorem 2 is in perfect agreement with the definition of the fractional Laplacian proposed by Ilić et al. [21] and based on the spectral mapping theorem.

From classical operator theory (Hutson [34]) the continuous standard Laplacian $(-\Delta)$ on $[0, L]$ coupled with homogeneous Neumann boundary conditions
345 has the set of orthonormal eigenfunctions $\{\phi_j\}_0^\infty$,

$$\phi_j(x) = w_j \cos\left(\frac{j\pi x}{L}\right), \text{ with } w_j = \sqrt{\frac{2}{L}} \text{ for } j \geq 1, w_0 = \frac{1}{\sqrt{L}}, \quad (25)$$

and corresponding eigenvalues $\nu_j = \left(\frac{j\pi}{L}\right)^2$ for all $j \geq 0$. Let \mathcal{H} be the Hilbert space $\mathcal{L}_2(0, L)$. Since the set of eigenfunctions $\{\phi_j\}_0^\infty$ forms a basis for \mathcal{H} , all $f \in \mathcal{H}$ can be written as a linear combination of the ϕ_j with coefficients \hat{f}_j
350 defined as the inner product of f and ϕ_j in \mathcal{H} .

By using the spectral mapping theorem [34], we can define the value of the operator $g(-\Delta)$, for a suitable continuous function g , in terms of the eigenvalue decomposition of $(-\Delta)$ as

$$g(-\Delta)f = \sum_{j=0}^{\infty} g(\nu_j) \hat{f}_j \phi_j, \quad \forall f \in \mathcal{H} \quad (26)$$

(provided that the series on the right-hand side of equation (26) converges), and
 355 conclude that the eigenvalues of $g(-\Delta)$ are the elements of the set $\{g(\nu_j)\}_0^\infty$,
 with $\{\phi_j\}_0^\infty$ the set of corresponding eigenfunctions. When $g(-\Delta) := (-\Delta)^{\alpha/2}$
 for $\alpha \in (1, 2]$, we find the spectral definition of the fractional power of the
 one-dimensional continuous Laplacian on the insulated finite interval.

Remark 2. *The operators $A_{\alpha,h}$ and $B_{\alpha,h}$ are both finite-dimensional approxi-*
 360 *mations of the continuous fractional Laplacian defined via its spectral decompo-*
sition.

The set of asymptotic values given by Theorem 2 for the spectrum of both
 operators indeed coincide with the fractional powers $\nu_j^{\alpha/2}$, where the ν_j are the
 eigenvalues of the standard continuous Laplacian on $[0, L]$, coupled to homoge-
 365 neous Neumann boundary conditions. Moreover, the common set of eigenvectors
 $\{\varphi_j\}_0^N$ of $A_{\alpha,h}$ and $B_{\alpha,h}$ can be viewed as the discretisation of the first $N + 1$
 orthogonal eigenfunctions $\{\phi_j\}_0^\infty$ of the continuous Laplacian, with a corrected
 normalisation coefficient defined so that $\|\varphi_j\|_2 = 1, \forall j$. Note that this asymp-
 totic result remains valid also when the discrete Laplacian B (on which the
 370 MTT definition of $B_{\alpha,h}$ is based) is obtained via a finite-difference scheme with
 first order approximation of the first order derivative at both ends of $[0, L]$.

Remark 3. *If the solution of a space-fractional equation on an insulated fi-*
nite domain $[0, L]$ is approximated via the method of lines, the use of either
 $A_{\alpha,h}$ or $B_{\alpha,h}$ leads essentially to the same result, provided that the number of
 375 *discretisation nodes of the spatial mesh is sufficiently high.*

Theorem 2 provides the link between the reflection strategy and the MTT,
 establishing the practical equivalence of the two approaches and proving the
 efficacy of the MTT in producing the correct solution to a space-fractional
 problem coupled to reflecting boundary conditions on a finite interval.

380 **Remark 4.** *The presented results suggest the use of a spectral approach, where*
the eigenvalues and eigenfunctions are defined according to the spectral mapping

theorem, as the natural approach to compute the solution of a space-fractional differential equation on an insulated finite interval.

The use of spectral techniques to compute the solution of fractional partial differential equations (FPDEs) is not new. Spectral methods for the discretisation of fractional order operators have been recently developed, for example, by Khader [35] for fixed order FPDEs involving the Caputo fractional derivative, by Bueno-Orovio et al. [36] in the case of the one-dimensional fractional Laplacian, and even for variable order FPDEs as in the work of Zayernouri and Karniadakis [37]. However, in all these cases the space-fractional operator is essentially coupled with standard homogeneous Dirichlet boundary conditions. Here, we focus on reflecting boundary conditions for $[0, L]$ and introduce the spectral technique to deal in a natural manner with the non-local operator defined via its eigenvalue/eigenfunction decomposition and obtain an infinite series representation of the solution. Moreover, the use of the spectral decomposition of the continuous limiting operator instead of the eigenpairs of the reflection matrix guarantees faster convergence to the exact solution of the non-local problem than in the case of the method of lines. A simple example of this faster convergence is given as follows.

Let us consider the space-fractional diffusion equation

$$\partial_t u = -(-\Delta)^{\alpha/2} u \quad (27)$$

on an insulated finite domain $[0, L]$, for $t > 0$, coupled with a given initial condition $u(x, 0)$. Without loss of generality, we have assumed $\mathcal{K}_\alpha = 1$.

Let $\mathbf{u}(t) = [u_0(t), u_1(t), \dots, u_N(t)]^T$ be the vector of solution approximations on a spatial grid of $N + 1$ nodes $x_i = ih$ with $h = \frac{L}{N}$, and let $A_{\alpha,h}$ be the reflection matrix constructed on the considered mesh. Then, by applying the method of lines to equation (27), we obtain the following system of ordinary differential equations:

$$\frac{d\mathbf{u}(t)}{dt} = -A_{\alpha,h}\mathbf{u}(t), \quad (28)$$

coupled to the initial vector $\mathbf{u}(0)$ obtained by evaluating $u(x, 0)$ on the spatial

mesh. Equation (28) can be integrated exactly in time leading to the solution

$$\mathbf{u}(t) = e^{-A_{\alpha,h}t} \mathbf{u}(0), \quad (29)$$

410 where the matrix exponential can be computed from a diagonalisation of $A_{\alpha,h}$ as

$$e^{-A_{\alpha,h}t} = V E V^{-1},$$

with $E := \text{diag}(e^{-\mu_0 t}, e^{-\mu_1 t}, \dots, e^{-\mu_N t})$, $V = [\varphi_0 | \dots | \varphi_N]$, and for all j , μ_j and φ_j defined as in Theorem 1.

On the other hand, if we look for the solution $u(x, t)$ of equation (27) via
415 the spectral method, then $u(x, t) = \sum_{j=0}^{\infty} \hat{u}_j(t) \phi_j(x)$ where the ϕ_j are as in equation (25). Recalling that

$$(-\Delta)^{\alpha/2} u(x, t) = \sum_{j=0}^{\infty} \nu_j^{\alpha/2} \hat{u}_j(t) \phi_j(x),$$

and using the orthonormality of the eigenfunctions ϕ_j , we see that for all j

$$\frac{d\hat{u}_j(t)}{dt} = -\nu_j^{\alpha/2} \hat{u}_j(t).$$

Hence, via exact integration in time, $\hat{u}_j(t) = e^{-\nu_j^{\alpha/2} t} \hat{u}_j(0)$, and the solution u can be written for all $x \in [0, L]$ and $t > 0$ as

$$u(x, t) = \sum_{j=0}^{\infty} e^{-\nu_j^{\alpha/2} t} \hat{u}_j(0) \phi_j(x). \quad (30)$$

420 Note that equation (30) is exact in both space and time. However, this expression involves an infinite sum and for practical reasons we truncate this sum after a certain number of terms, $j = j_{\max}$, and only consider a finite number of eigenfunctions in the solution expansion. In addition, for a generic initial condition $u(x, 0)$, we have to introduce a suitable numerical integration scheme
425 to approximate the integral coefficients $\hat{u}_j(0) = \int_0^L u(x, 0) \phi_j(x) dx$.

Here, we choose to compute the solution (30) on the same grid used for the reflection approach. We truncate the sum in equation (30) after the first $N + 1$ terms and approximate the value of each $\hat{u}_j(0)$ via the trapezoidal rule with nodes $x_i = i h$, with $h = \frac{L}{N}$.

430 In Figure 2 we plot the error made at a given $t = \bar{t} > 0$ by computing the so-
 lutions (29) and (30) with the same initial condition, $u(x, 0) = \frac{3}{5-4\cos(x)}$, but for
 different values of N and $\alpha \in (1, 2]$. The error for both approaches is computed
 as $\|u - u_{\text{ref}}\|_{\infty}$, where u_{ref} is a reference solution computed from equation (30)
 with $j_{\text{max}} = 1000$ and global adaptive quadrature for the numerical integration
 435 of $\hat{u}_j(0)$ for all j , $0 \leq j \leq j_{\text{max}}$.

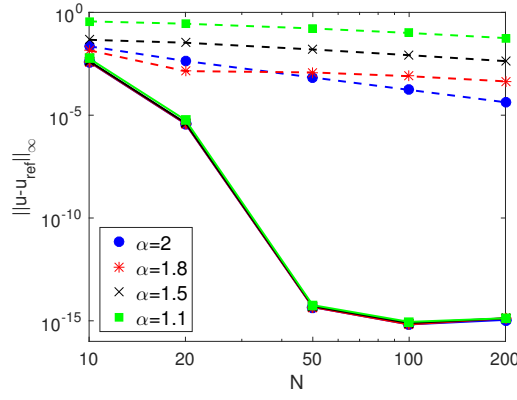


Figure 2: Log-log plot of the error made in the approximation of the solution to equation (27) with initial condition $u(x, 0) = \frac{3}{5-4\cos(x)}$, when the reflection matrix (dashed lines) or the spectral method (continuous lines) are used, respectively. For both methods the solution is computed at $\bar{t} = 1$ on the insulated interval $[0, 2\pi]$ with $N = 10, 20, 50, 100, 200$ ($N + 1$ is the total number of nodes in the spatial mesh). The marker of each line identifies the order α . Linear interpolation is used to facilitate visualisation.

As the value of N increases, the error made in the solution approximation decreases. However, there is a substantial difference between the two solution strategies. When the reflection matrix is used, the logarithm of the error, $\log \|u - u_{\text{ref}}\|_{\infty}$, is a decreasing linear function of $\log N$, leading to $\|u - u_{\text{ref}}\|_{\infty} = \mathcal{O}(h^c)$, for some constant $c > 0$, whose value depends on the fractional order α . On the other hand, the spectral method produces a much more accurate solution approximation and due to the regularity of the initial condition and its derivatives at the boundaries of the considered interval (ensuring geometric decay of the integral coefficients involved in the spectral decomposition of

the solution), the error decays exponentially until machine precision is reached. This technique can then be used to solve fractional reaction-diffusion equations on bounded domains where there is a nonlinear source term.

4.3. Fractional flux at boundary nodes

We conclude this section by analysing the behaviour of the approximation to our modified definition of fractional flux (15) at the boundary nodes of the considered finite domain for $N \rightarrow \infty$.

Using similar arguments to the ones made in the proof of the main theorem for $r = 1, \dots, N-1$ (see Supplementary Material) from equation (18) we obtain

$$\begin{aligned} g_r + g_{2N-r} &= \frac{1}{2N} \sum_{l=1}^{2N-1} \left(e^{-\frac{ilr\pi}{N}} + e^{\frac{ilr\pi}{N}} \right) \left(1 - e^{\frac{il\pi}{N}} \right)^{\alpha-1} \\ &= \frac{1}{2N} \sum_{l=1}^{2N-1} 2 \cos \left(\frac{lr\pi}{N} \right) \left(1 - e^{\frac{il\pi}{N}} \right)^{\alpha-1} \end{aligned}$$

and by exploiting the definition of fractional power of a complex number (Definition 3 of Supplementary Material) and various elementary properties of basic trigonometric functions we obtain

$$\begin{aligned} g_r + g_{2N-r} &= \frac{2^{\alpha-1}}{N} \left[\sum_{l=1}^{N-1} 2 \cos \left(\frac{lr\pi}{N} \right) \left(\sin \frac{l\pi}{2N} \right)^{\alpha-1} \cos \left(\frac{(\alpha-1)(N-l)\pi}{2N} \right) \right. \\ &\quad \left. + \cos(r\pi) \right]. \end{aligned}$$

Similarly, we have

$$\begin{aligned} g_0 &= \frac{2^{\alpha-2}}{N} \left[\sum_{l=1}^{N-1} 2 \left(\sin \frac{l\pi}{2N} \right)^{\alpha-1} \cos \left(\frac{(\alpha-1)(N-l)\pi}{2N} \right) + 1 \right], \\ g_N &= \frac{2^{\alpha-2}}{N} \left[\sum_{l=1}^{N-1} 2 \cos(l\pi) \left(\sin \frac{l\pi}{2N} \right)^{\alpha-1} \cos \left(\frac{(\alpha-1)(N-l)\pi}{2N} \right) + \cos(N\pi) \right]. \end{aligned}$$

Therefore, once the numerical solution vector $u(t) = [u_0, u_1, \dots, u_N]^T$ has been computed at a given $t > 0$, using the above expression of the various coefficients g_r we can calculate $\frac{1}{h^{\alpha-1}} \sum_{k=0}^N M_{0,k} u_k$ and observe the behaviour of this quantity as $N \rightarrow \infty$.

We consider the following two cases and make some important remarks:

- **Case $\alpha = 2$.** It is immediate to see that when $\alpha - 1 = 1$, the sum in (16) only involves u_0 and u_1 . In particular, we obtain that $g_0 = 1$, $g_1 + g_{2N-1} = -1$ and all other $g_r = 0$, independently from the number of nodes considered for the spatial discretisation of the interval $[0, L]$. Expression (16) becomes

$$\lim_{h \rightarrow 0^+} \frac{u_0 - u_1}{h}, \quad (31)$$

which is a first order approximation of the derivative $\frac{\partial u}{\partial x}$ at $x = 0$. Similarly, the approximation of the left fractional flux at $x = L$ reduces to a first order approximation of the derivative $\frac{\partial u}{\partial x}$ in terms of u_N and u_{N-1} . From our numerical tests we see that $\forall t$, as $N \rightarrow \infty$ the limit (31) goes to zero (as the one at $x = L$ does), thus showing that our solution satisfies homogeneous Neumann boundary conditions at both boundaries of the considered domain.

- **Case $\alpha < 2$.** Not having imposed any condition on the fractional flux, we expect the solution to our fractional differential equation on $[0, L]$ to be such that $D_{-x}^{\alpha-1} u \Big|_{x=0} \neq 0$. This is indeed what we see from our numerical simulations by evaluating $\frac{1}{h^{\alpha-1}} \sum_{k=0}^N M_{0,k} u_k(t)$ at different time points t and for increasing values of N . In particular, for a fixed t the considered quantity converges to a non-zero value as $N \rightarrow \infty$ indicating that the fractional flux at the origin is not vanishing in the general case. However, we notice that this quantity is a decreasing function of time, and in the limit for $t \rightarrow \infty$ we find that $\frac{1}{h^{\alpha-1}} \sum_{k=0}^N M_{0,k} u_k(t) \rightarrow 0$. In fact, the solution to our problem converges to the constant function equal to the mass of the initial condition on the entire spatial domain, and for a constant solution vector with $u_k = \bar{u}$ for all k , we simply have

$$\sum_{k=0}^N M_{0,k} u_k = \bar{u} \sum_{r=0}^{2N-1} g_r \equiv 0$$

where the second sum can be shown to be identically equal to zero by using elementary properties of basic trigonometric functions and Lagrange's theorem for the sum of cosines.

Once again, similar considerations can be made for the modified fractional flux at the other end, $x = L$, of the finite interval.

5. Discussion and conclusions

In this paper we prove that the discrete fractional Laplacian defined via the MTT is indeed a valid approach for the computation of the solution to a space-fractional equation on an insulated finite interval. The spectrum of the operator defined by raising to a fractional power the standard discrete Laplacian coupled to homogeneous Neumann boundary conditions in fact converges to the same limit obtained for the spectrum of another discrete operator derived from the theory of α -stable symmetric Lévy flights, here referred to as the reflection matrix. This shows that, in the limit, the two approaches lead to the same result, ensuring the correct representation of reflecting boundary conditions for the fractional problem on the considered finite interval.

We strongly believe that this result will hold in more than one spatial dimension with regular and possibly irregular bounded domains, but to the best of our knowledge, a formal proof is yet to be established. Generalising this result to more than one spatial dimension is indeed a complex task. In order to obtain the analytic representation of the operator embedding reflecting boundary conditions in Section 2 we used the fact that $-(-\Delta)^{\alpha/2} = \mathcal{R}_x^\alpha$ in \mathbb{R} . However, this relationship does not hold in \mathbb{R}^n , $n > 1$. In more than one spatial dimension, the continuous fractional Laplacian can be represented as an hypersingular integral as shown by Samko et al. [14]. However, to obtain a multidimensional analogue of the reflection matrix defined in Section 3, we would need to introduce a finite-difference representation of this integral operator and how to do this is certainly not straightforward. Moreover, the formalisation of the concept of reflective boundaries in \mathbb{R}^n , $n > 1$, poses the challenge of defining the trajectory of a bouncing particle hitting a possibly curved or irregular reflecting wall (depending on the boundary of the spatial domain) with an *a priori* undefined angle of incidence. Perhaps some progress towards the finite-

515 difference representation of the multidimensional fractional Laplacian could be
 made along the lines of the work proposed by del Teso and Vázquez [38], and
 possibly greater insight into the idea of reflections could be gained from the work
 of Tabachnikov [39] on billiards trajectories in various geometries. However, the
 connection between these two ideas is not obvious to us at this stage and hence,
 520 we leave this discussion as a research focus of our future investigation.

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Appendix A. Macroscopic equation for P_∞

Let $\hat{f}(k)$ and $\tilde{h}(u)$ denote the Fourier and Laplace transforms of functions
 530 $f(x)$ and $h(t)$ of $x \in \mathbb{R}$ and $t \in \mathbb{R}^+$, respectively. From equation (4), we find
 that, in Fourier–Laplace variables,

$$\hat{P}_\infty(k, u) = \hat{g}_0(k) \left(\frac{1 - \tilde{\psi}_{\tau_0}(u)}{u} \right) + \hat{P}_\infty(k, u) \hat{\phi}_l(k) \tilde{\psi}_{\tau_0}(u). \quad (\text{A.1})$$

By computing the Fourier and Laplace transforms of $\phi_l(x)$ and $\psi_{\tau_0}(t)$, we ob-
 tain $\hat{\phi}_l(k) = e^{-l^\alpha |k|^\alpha}$ and $\tilde{\psi}_{\tau_0}(u) = (\tau_0 u + 1)^{-1}$, respectively. Therefore, equa-
 tion (A.1) can be rewritten as

$$u \hat{P}_\infty(k, u) - \hat{g}_0(k) = \hat{P}_\infty(k, u) \frac{e^{-l^\alpha |k|^\alpha} - 1}{\tau_0}. \quad (\text{A.2})$$

535 For fixed k and u , in order to obtain the macroscopic behaviour of P_∞ , we
 consider equation (A.2) in the limit $(l, \tau_0) \rightarrow (0, 0)$, while keeping the ratio
 l^α/τ_0 constant (namely, $l^\alpha/\tau_0 = K_\alpha$). As a result

$$u \hat{P}_\infty(k, u) - \hat{g}_0(k) = -K_\alpha |k|^\alpha \hat{P}_\infty(k, u),$$

and hence, by inverting the transforms, we see that on \mathbb{R} , P_∞ is the solution of the fractional diffusion equation (5).

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