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NUMERICAL APPROXIMATION OF A FRACTIONAL-IN-SPACE DIFFUSION EQUATION, I *

M. Ilic, F. Liu, I. Turner and V. Anh

Abstract

This paper provides a new method and corresponding numerical schemes to approximate a fractional-in-space diffusion equation on a bounded domain under boundary conditions of the Dirichlet, Neumann or Robin type. The method is based on a matrix representation of the fractional-in-space operator and the novelty of this approach is that a standard discretisation of the operator leads to a system of linear ODEs with the matrix raised to the same fractional power. Numerical results are provided to gauge the performance of the proposed method relative to exact analytical solutions determined using a spectral representation of the fractional derivative. Initial results for a variety of one-dimensional test problems appear promising. Furthermore, the proposed strategy can be generalised to higher dimensions.

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1. Introduction

In the Eulerian theory of turbulence, a concentration field $\varphi(t,\mathbf{x})$ is commonly assumed to satisfy the advection-diffusion equation

$$\frac{\partial\varphi}{\partial t}+\nabla.(\mathbf{u}\varphi)=\kappa\Delta\varphi(t,\mathbf{x}),\quad t\in\mathbb{R}_+,\,\mathbf{x}\in D\subset\mathbb{R}^n, \tag{1.1}$$

where ∇ is the gradient vector, $\mathbf{u}(t,x)$ is the velocity vector field, κ is the molecular diffusivity coefficient and Δ is the Laplacian. On the other hand, in the Lagrangian theory, the assumptions of model (1.1) are equivalent to assuming that the particle trajectories $\mathbf{x}(t)$ satisfy the Itô stochastic differential equation

$$d\mathbf{x}(t)=\mathbf{u}(t,\mathbf{x}(t))\,dt+(2\kappa)^{1/2}\,d\mathbf{B}(t),$$

where the components of $\mathbf{B}(t)$ are independent Brownian motions (Schuss [25], Thomson [29]). In the context of anomalous diffusion, particularly under long-range dependence, the equivalence between the Eulerian and Lagrangian approaches has not been established.

A fundamental example of a fractional-in-space diffusion equation is

$$\frac{\partial\varphi}{\partial t}=-\kappa(-\Delta)^{\alpha}\varphi(t,\mathbf{x}),\,\alpha>0, \tag{1.2}$$

where $(-\Delta)^{\alpha}$ is understood as the inverse of the Riesz potential defined by the kernel

$$J_{\alpha}(\mathbf{x})=\frac{\Gamma(n/2-\alpha)}{\pi^{n/2}4^{\alpha}\Gamma(\alpha)}\,|\mathbf{x}|^{2\alpha-n}$$

(Stein [26]). For $\alpha\in(0,1]$ the Green's function of (1.2) is the symmetric $2\alpha-$stable probability density function and the corresponding particle trajectories follow a symmetric $2\alpha-$stable Lévy motion. This provides a Lagrangian interpretation of the fractional diffusion equation (1.2) (see Bochner [5], also Feller [8] for an extension to the asymmetric case). In fact, Feller [8] considered the problem of generating all the stable probability distributions through the semigroup (known as the Feller semigroup) generated by the Green's function of the diffusion equation

$$\frac{\partial\varphi}{\partial t}=\mathcal{D}_{\theta}^{2\alpha}\varphi(t,\mathbf{x}),\;t>0,\,\mathbf{x}\in\mathbb{R}, \tag{1.3}$$

where $\mathcal{D}_{\theta}^{2\alpha}$ is the pseudo-differential operator with symbol

$$\widehat{\mathcal{D}_{\theta}^{2\alpha}}=-|\lambda|^{2\alpha}\exp(i\,\mathrm{sign}(\lambda)\,\theta\pi/2),$$

α being the index of stability and θ the index of skewness (asymmetry). When $\theta = 0$, (1.3) is reduced to (1.2) with $\kappa = 1$, and the Feller semigroup represents all 2α-stable distributions.

Eq. (1.2) and its extensions have been treated by many authors including Schneider and Wyss [28], Schneider [24], Kochubei [13], Mainardi [21], Saichev and Zaslavsky [27], Gorenflo *et al.* [11, 12, 10], Anh and Leonenko [2, 3, 4].

Analytical solutions for equations of the type (1.2) using transform methods on unbounded domains are known for some cases (see Schneider and Wyss [28], for example). For bounded domains and under some boundary conditions, it appears that the problem must be approached via numerical methods. To be precise one wants to solve Eq. (1.2) on a bounded domain D and under a variety of boundary conditions of the Dirichlet, Neumann and Robin types, viz.

(i) $\varphi = f$ on ∂D (Dirichlet);
(ii) $\frac{\partial \varphi}{\partial n} := (\mathbf{n} \cdot \nabla)\varphi = f$ on ∂D (with $\mathbf{n}$ outer normal) (Neumann);
(iii) $\frac{\partial \varphi}{\partial n} + \beta\varphi = f$ on ∂D, $\beta > 0$ (Robin).

In this paper we will provide a method and corresponding numerical schemes to approximate the solution of Eq. (1.2) in one dimension subject to one of these boundary condition types with $f = 0$ (the so-called homogeneous boudary conditions). The nonhomogeneous boundary conditions will be discussed in a subsequent paper by the authors. Specifically, an approximate solution is sought for the following problem:

PROBLEM 1. *Solve the following boundary value problem (BVP) in one dimension:*

$$\frac{\partial \varphi}{\partial t} = -\kappa \left(-\frac{\partial^2}{\partial x^2} \right)^{\frac{\alpha}{2}} \varphi, \quad 0 < x < L, \tag{1.4}$$

with the initial condition

$$\varphi(x, 0) = g(x)$$

together with one of the following boundary conditions:

(i) $\varphi(0, t) = 0, \quad \varphi(L, t) = 0 \ldots (BC)_1$;
(ii) $\varphi_x(0, t) = 0, \quad \varphi_x(L, t) = 0 \ldots (BC)_2$;
(iii) $\varphi_x(0, t) + \beta\varphi(0, t) = 0, \quad \varphi_x(L, t) + \beta\varphi(L, t) = 0 \ldots (BC)_3$.

The solutions of Problem 1 will be compared using three methods. In Section 2, the fractional derivative is expressed using the integral representation. In Section 3, the fractional derivative is expressed using the spectral

representation. In Section 4, a new approach is formulated using the finite difference method to approximate the fractional derivative by a matrix representation.

For many years the finite difference method has been a mainstay in the numerical treatment of partial differential equations (Morton and Mayers [20]). To illustrate the idea, consider the simplest diffusion equation (with constant diffusivity κ) in one dimension:

$$\begin{aligned} \frac{\partial \varphi}{\partial t} &= \kappa \frac{\partial^2 \varphi}{\partial x^2}, \quad 0 < x < 1, \\ \varphi(0,t) &= f_1(t), \ \varphi(1,t) = f_2(t), \\ \varphi(x,0) &= g(x). \end{aligned} \tag{1.5}$$

Introducing a finite difference approximation, we obtain

$$\begin{aligned} \frac{d\varphi_i}{dt} &= \frac{\kappa}{h^2}(\varphi_{i+1} - 2\varphi_i + \varphi_{i-1}), \quad (i = 1, \cdots, N-1), \\ \varphi_0 = f_1(t), &\qquad \varphi_N = f_2(t), \\ \varphi(x_i, 0) &= g(x_i), \quad (i = 1, \cdots, N-1), \end{aligned}$$

where $\varphi_i = \varphi(x_i, t)$, h is the space step defined as $h = \frac{1}{N}$.

The above equations can be expressed as the following system of ordinary differential equations:

$$\frac{d\mathbf{\Phi}}{dt} = -\eta \mathbf{A}\mathbf{\Phi} + \mathbf{b}, \tag{1.6}$$

where $\eta = \frac{\kappa}{h^2}$ and $\mathbf{\Phi}, \mathbf{b} \in \mathbb{R}^{N-1}$, $\mathbf{A} \in \mathbb{R}^{N-1 \times N-1}$,

$$\mathbf{\Phi} = \begin{bmatrix} \varphi_1 \\ \vdots \\ \varphi_{N-1} \end{bmatrix}, \mathbf{b} = \begin{bmatrix} \eta\varphi_0 \\ 0 \\ \vdots \\ 0 \\ \eta\varphi_N \end{bmatrix}, \mathbf{A} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

The matrix $\mathbf{A}$ is a symmetric positive definite (SPD) matrix. Initially, we have

$$\mathbf{\Phi}(0) = [g(h), g(2h), \ldots, g((N-1)h)]^T. \tag{1.7}$$

We make an important observation: If $\mathbf{b} = \mathbf{0}$ (i.e. homogeneous boundary conditions) and if the operator $T = -\frac{\partial^2}{\partial x^2}$ has a matrix representation $m(T)$,

then Eq.(1.5) becomes

$$\frac{dm(\varphi)}{dt} = -\kappa m(T)m(\varphi),$$

where m is the "coordinate" isomorhism $\varphi \leftrightarrow \mathbf{\Phi}$. In other words $\frac{1}{h^2}\mathbf{A} \approx m(T)$, i.e., $\frac{1}{h^2}\mathbf{A}$ is an approximate matrix representation of T.

The aim of this study is to explore the possibility that Eq. (1.4) can be replaced by

$$\frac{d\mathbf{\Phi}}{dt} = -\bar{\eta}\mathbf{A}^{\frac{\alpha}{2}}\mathbf{\Phi},$$

where $\bar{\eta} = \frac{\kappa}{h^\alpha}$ for homogeneous boundary conditions. Numerical results are obtained to evaluate the performance of the proposed method relative to exact analytical solutions. The method also can be extended in a natural manner to higher dimensions, which is an advantage over existing techniques.

2. Integral representation of fractional derivative

2.1. Caputo fractional derivative

A fractional-in-space diffusion equation may take the form

$$\frac{\partial \varphi}{\partial t} = k {}_a^c D_x^\alpha \varphi, \quad a < x < b, \tag{2.1}$$

where ${}_a^c D_x^\alpha$ denotes the fractional derivative in the Caputo sense:

$${}_a^c D_x^\alpha \varphi(x) = \frac{1}{\Gamma(n-\alpha)} \int_a^x [\frac{\partial^n \varphi(\xi)}{\partial \xi^n}] \frac{d\xi}{(x-\xi)^{\alpha-n+1}}, \quad (n-1 < \alpha < n).$$

Let $h = (b-a)/N$, $x = x_l = a + lh$, $\varphi_0 = \varphi(x - lh) = \varphi(a)$, $\varphi_1 = \varphi(x-(l-1)h) = \varphi(a+h)$,...,$\varphi_{l-j} = \varphi(x-jh)$,...,$\varphi_l = \varphi(x) = \varphi(a+lh)$. Then the fractional derivative term with $n = 2$ can be approximated by [19, 20]

$$\begin{aligned} {}_a^c D_x^\alpha \varphi(x) &= \frac{1}{\Gamma(2-\alpha)} \int_a^x \frac{\varphi^{(2)}(\xi) d\xi}{(x-\xi)^{\alpha-1}} \\ &= \frac{1}{\Gamma(2-\alpha)} \int_0^{x-a} \frac{\varphi^{(2)}(x-\xi) d\xi}{\xi^\alpha} \end{aligned}$$

$$= \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{l-1} \int_{jh}^{(j+1)h} \frac{\varphi^{(2)}(x-\xi)d\xi}{\xi^{\alpha-1}}$$

$$= \frac{1}{\Gamma(2-\alpha)} \sum_{j=0}^{l-1} \frac{\varphi(x-(j-1)h) - 2\varphi(x-jh) + \varphi(x-(j+1)h)}{h^2} \times \int_{jh}^{(j+1)h} \frac{d\xi}{\xi^{\alpha-1}}$$

$$= \frac{h^{-\alpha}}{\Gamma(3-\alpha)} \sum_{j=0}^{l-1} (\varphi_{l-j+1} - 2\varphi_{l-j} + \varphi_{l-j-1})[(j+1)^{2-\alpha} - j^{1-\alpha}].$$

Using the technique outlined in Liu *et al.* [19, 20], equation (2.1) can be recast into the following ordinary differential equation (ODE):

$$\frac{d\varphi_l}{dt} = \frac{k}{h^\alpha \Gamma(3-\alpha)} \sum_{j=0}^{l-1} (\varphi_{l-j+1} - 2\varphi_{l-j} + \varphi_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}],$$

$l = 1, 2, ..., N$, where $\varphi_l = \varphi(x_l, t)$.

2.2. Riesz fractional derivative

A fractional-in-space diffusion equation may also be written as

$$\frac{\partial \varphi}{\partial t} = {}_0^R D_x^\alpha \varphi, \quad a < x < b, \tag{2.2}$$

where ${}_0^R D_x^\alpha$ denotes the Riesz fractional derivative

$${}_0^R D_x^\alpha = -(-\triangle)^{\frac{\alpha}{2}} = \frac{d^\alpha}{d|x|^\alpha} = -{}_x I_0^{-\alpha}$$

and

$${}_x I_0^{-\alpha} \varphi(x) = C_-(\alpha) {}_x I_+^\alpha \varphi(x) + C_+(\alpha) {}_x I_-^\alpha \varphi(x).$$

Here, ${}_x I_\pm^{-\alpha}$ denote the Riemann-Liouville fractional integrals, also known as Weyl fractional integrals, which are defined as

$${}_x I_+^{-\alpha} \varphi(x) = \frac{1}{\Gamma(\alpha)} \int_a^x \frac{\varphi(\xi)d\xi}{(x-\xi)^{1-\alpha}},$$

$$ {}_xI_-^{-\alpha}\varphi(x) = \frac{1}{\Gamma(\alpha)}\int_x^b \frac{\varphi(\xi)d\xi}{(\xi-x)^{1-\alpha}},$$
$$ C_-(\alpha) = C_+(\alpha) = \frac{1}{2\cos(\frac{\pi\alpha}{2})},$$

and thus we recover the Riesz potential

$$ {}_xI_0^{-\alpha}\varphi(x) = \frac{1}{2\Gamma(\alpha)\cos(\frac{\pi\alpha}{2})}\int_a^b \frac{\varphi(\xi)d\xi}{|x-\xi|^{1-\alpha}}.$$

We define by analytic continuation the pseudo-differential operator in the whole range $1 < \alpha < 2$ as

$$ {}_xD_0^{\alpha} = -(C_+(\alpha){}_xD_+^{\alpha} + C_-(\alpha){}_xD_-^{\alpha}).$$

For integral representations of the operators ${}_xI_{\pm}^{\alpha}$, we have

$$ {}_xI_{\pm}^{\alpha} = \frac{d^2}{dx^2}({}_xI_{\pm}^{2-\alpha}).$$

Therefore,

$$\begin{aligned} {}_xD_+^{\alpha}\varphi &= \frac{d^2}{dx^2}({}_xI_+^{2-\alpha})\varphi \\ &= \frac{\varphi(a)(x-a)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{\varphi'(a)(x-a)^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\int_a^x \frac{\varphi^{(2)}(\xi)d\xi}{(x-\xi)^{\alpha-1}}, \end{aligned}$$

$$\begin{aligned} {}_xD_-^{\alpha}\varphi &= \frac{d^2}{dx^2}({}_xI_-^{2-\alpha})\varphi \\ &= \frac{\varphi(b)(b-x)^{-\alpha}}{\Gamma(1-\alpha)} - \frac{\varphi'(b)(b-x)^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\int_x^b \frac{\varphi^{(2)}(\xi)d\xi}{(\xi-x)^{\alpha-1}}. \end{aligned}$$

Using the technique in Liu *et al.* [19, 20], equation (2.2) can be recast into the following ODE:

$$\begin{aligned} \frac{d\varphi_l}{dt} = -\frac{1}{2\Gamma(\alpha)\cos(\frac{\pi\alpha}{2})}\frac{kh^{-\alpha}}{\Gamma(3-\alpha)}\Bigg\{ & \frac{(1-\alpha)(2-\alpha)\varphi_0}{l^{\alpha}} \\ + \frac{(2-\alpha)}{l^{\alpha-1}}(\varphi_1-\varphi_0) + \sum_{j=0}^{l-1}(\varphi_{l-j+1} - 2\varphi_{l-j} + \varphi_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}] & \\ + \frac{(1-\alpha)(2-\alpha)\varphi_N}{(N-l)^{\alpha}} - \frac{(2-\alpha)}{(N-l)^{(\alpha-1)}}(\varphi_N - \varphi_{N-1}) & \\ + \sum_{j=0}^{N-l-1}(\varphi_{l+j-1} - 2\varphi_{l+j} + \varphi_{l+j+1})[(j+1)^{2-\alpha} - j^{2-\alpha}]\Bigg\}. & \end{aligned}$$

2.3. Method of lines

The method of lines (MOL) is a well-known technique for solving parabolic-type partial differential equations [30]. In the MOL, time integration is accomplished using an ODE or a differential-algebraic equations (DAE) integrator. Some of the mathematical and numerical difficulties in working with these approaches include error control, solution-order adjustment, time-step adjustment, and nonlinear and linear algebraic equation resolution. Brenan *et al.* [7] developed the differential/algebraic system solver (DASSL), which is based on the backward difference formulas (BDF). DASSL approximates the derivatives using the k-th order BDF, where k ranges from one to five. At every step, it chooses the order k and step size based on the behaviour of the solution. In this work, we use DASSL as our ODE solver. This technique has been used to solve adsorption problems involving step gradients in bidisperse solids [14, 17], hyperbolic models of transport in bidisperse solids [15], transport problems involving steep concentration gradients [16], and modelling saltwater intrusion into coastal aquifers [18].

3. Spectral representation

Let H be the real Hilbert space $\mathcal{L}_2(0, L)$ with the usual inner product. Consider the operator $T : \mathcal{H} \to H$ defined by $T\varphi = -\frac{d^2\varphi}{dx^2} = -\triangle\varphi$ on

$$\mathcal{H} = \left\{\varphi \in H;\ \varphi' \text{ is absolutely continuous}, \varphi', \varphi'' \in \mathcal{L}_2(0, L),\ \mathcal{B}(\varphi) = 0\right\},$$

where $\mathcal{B}(\varphi)$ is one of the boundary conditions in Problem 1. It is known that T is a closed, self-adjoint operator whose eigenfunctions $\{\varphi_n\}_{n=1}^{\infty}$ form an orthonormal basis for H. Thus $T\varphi_n = \lambda_n\varphi_n,\ n = 1, 2, \cdots$. For any $\varphi \in H$,

$$\varphi = \sum_{n=1}^{\infty} c_n\varphi_n, \quad c_n =< \varphi, \varphi_n >,$$

$$T\varphi = \sum_{n=1}^{\infty} \lambda_n c_n\varphi_n.$$

If ψ is a continuous function on $\mathbb{R}$, then

$$\psi(T)\varphi = \sum_{n=1}^{\infty} \psi(\lambda_n)c_n\varphi_n, \tag{3.1}$$

provided $\sum_{n=1}^{\infty} |\psi(\lambda_n)c_n|^2 < \infty$. Hence if the eigenvalue problem for T can be solved explicitly, then Problem 1 can be easily solved as shown by the following examples, where $\psi(t) = t^{\frac{\alpha}{2}}$.

Example 1. Solve the following one dimensional space fractional diffusion equation with given initial and boundary-value conditions

$$\begin{aligned} \frac{\partial \varphi}{\partial t} &= -\kappa(-\triangle)^{\frac{\alpha}{2}}\varphi, \quad 0 < x < L, && (3.2)\\ \varphi(0,t) &= \varphi(L,t) = 0, && (3.3)\\ \varphi(x,0) &= g(x). && (3.4) \end{aligned}$$

First we obtain the spectral representation of the operator T by solving the eigenvalue problem:

$$\begin{aligned} -\triangle y &= \lambda y,\\ y(0) &= 0, \quad y(L) = 0. \end{aligned}$$

The eigenvalues are $\lambda_n = \frac{n^2\pi^2}{L^2}$ for $n = 1, 2, \cdots$, and the corresponding eigenfunctions are nonzero constant multiples of $y_n(x) = \sin(\frac{n\pi x}{L})$.

Next set $\varphi(x,t) = \sum_{n=1}^{\infty} c_n(t)\sin(\frac{n\pi x}{L})$, which automatically satisfies the boundary condition (3.3). Using equation (3.1) and substituting $\varphi(x,t)$ into equation (3.2), we obtain

$$\sum_{n=1}^{\infty}[\frac{dc_n}{dt} + \kappa(\frac{n^2\pi^2}{L^2})^{\frac{\alpha}{2}}c_n]\sin(\frac{n\pi x}{L}) = 0.$$

The problem for c_n becomes

$$\frac{dc_n}{dt} + \kappa(\frac{n^2\pi^2}{L^2})^{\frac{\alpha}{2}}c_n = 0,$$

which has the general solution

$$c_n(t) = c_n(0)\exp(-\kappa(\frac{n^2\pi^2}{L^2})^{\frac{\alpha}{2}}t).$$

To obtain $c_n(0)$ we use the initial condition (3.4)

$$\varphi(x,0) = \sum_{n=1}^{\infty} c_n(0)\sin(\frac{n\pi x}{L}) = g(x).$$

This gives

$$c_n(0) = \frac{2}{L}\int_0^L g(\xi)\sin(\frac{n\pi\xi}{L})d\xi = b_n.$$

With this choice of the coefficients, we have the solution for the distribution function:

$$\varphi(x,t) = \sum_{n=1}^{\infty} b_n \sin(\frac{n\pi x}{L})\exp(-\kappa(\frac{n^2\pi^2}{L^2})^{\frac{\alpha}{2}}t).$$

Example 2. Solve the following fractional-in-space diffusion equation with radiating end $(BC)_3$ in one dimension:

$$\frac{\partial\varphi}{\partial t} = -\kappa(-\triangle)^{\frac{\alpha}{2}}\varphi, \quad 0 < x < 1, \tag{3.5}$$

$$\varphi(0,t) = 0, \quad \varphi'(1,t) + \varphi(1,t) = 0, \quad t > 0, \tag{3.6}$$

$$\varphi(x,0) = g(x). \tag{3.7}$$

The operator T, defined by

$$Ty = -\frac{d^2y}{dx^2}, \quad y(0) = 0, \quad y'(1) + y(1) = 0$$

has the eigenvalues λ_n, $n = 1, 2, \cdots$, which are the roots of the equation

$$\sin(\sqrt{\lambda}) + \sqrt{\lambda}\cos(\sqrt{\lambda}) = 0,$$

and can be found using a numerical method [6]. The corresponding normalized eigenfunctions are

$$\varphi_n(x) = \frac{\sqrt{2}\sin(\sqrt{\lambda_n}x)}{(1+\cos^2\sqrt{\lambda_n})^{\frac{1}{2}}}, \quad n = 1, 2, \cdots.$$

Next set $\varphi(x,t) = \sum_{n=1}^{\infty} c_n(t)\varphi_n(x)$ and substitute into Eq. (3.5) to obtain

$$\sum_{n=1}^{\infty}[\frac{dc_n}{dt} + \kappa\lambda_n^{\frac{\alpha}{2}}c_n]\varphi_n(x) = 0.$$

Solving the resulting ODE for $c_n(t)$ using the initial condition, we obtain

$$\varphi(x,t) = \sum_{n=1}^{\infty} c_n \frac{\sqrt{2}\sin(\sqrt{\lambda_n}x)}{(1+\cos^2\sqrt{\lambda_n})^{\frac{1}{2}}}\exp(-\lambda_n^{\frac{\alpha}{2}}\kappa t),$$

where

$$c_n = \int_0^1 g(x) \frac{\sqrt{2}\sin(\sqrt{\lambda_n}x)}{(1+\cos^2\sqrt{\lambda_n})^{\frac{1}{2}}} dx.$$

REMARK 1. For numerical calculations, an infinite series is typically approximated by a finite sum. That is, we set

$$\bar{\varphi} = \sum_{i=1}^{n} c_i \varphi_i.$$

It is still true that

$$T\bar{\varphi} = \sum_{i=1}^{n} \lambda_i c_i \varphi_i,$$

and

$$\psi(T)\bar{\varphi} = \sum_{i=1}^{n} \psi(\lambda_i) c_i \varphi_i.$$

One can think of this as working on a finite-dimensional invariant subspace $X_n = Span\{\varphi_1, \cdots, \varphi_n\} \subset H$, with the operator $T|_{X_n}$, which is the restriction of T to X_n. The difficulties arise when we don't know invariant subspaces of T and we have to work with noninvariant subspaces, for example, when diffusivity is nonconstant or geometry is not simple.

4. Matrix representation

Whereas bounded operators readily admit matrix representation on a separable Hilbert space, for unbounded, symmetric and closed operators like differential operators, care is required [1], but there do exist bases for matrix representation of such operators. If $\{\varphi_n\}_{n=1}^{\infty}$ is the eigenfunction orthonormal basis for H as discussed in Section 3, then we have the representation

$$\varphi \in H \leftrightarrow \mathbf{c} = (c_1, \cdots, c_n, \cdots)^T \in \ell_2,$$

i.e. $m(\varphi) = \mathbf{c}$, where m is the "coordinate" isomorphism. In this case,

$$m(T) = \mathbf{\Lambda} = diag(\lambda_i) \quad \text{and} \quad m(\psi(T)) = \psi(\mathbf{\Lambda}) \quad \text{or} \quad m(\psi(T)) = diag(\psi(\lambda_i)).$$

Let $X_n = Span\{\varphi_1, \cdots, \varphi_n\}$ be a finite-dimensional subspace of H. Then $X_n \subset X_{n+1}$ and $\bigcup_{n=1}^{\infty} X_n$ is dense in H. Since X_n is an invariant subspace of T, we have for $\bar{\varphi} \in X_n$, $m(\bar{\varphi}) = \mathbf{c} = (c_1, \cdots, c_n)^T$,

$$m(T) = \mathbf{\Lambda} = \begin{bmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{bmatrix},$$

and

$$m(\psi(T)) = \psi(\mathbf{\Lambda}) = \begin{bmatrix} \psi(\lambda_1) & & & \\ & \psi(\lambda_2) & & \\ & & \ddots & \\ & & & \psi(\lambda_n) \end{bmatrix}.$$

In general, if X_n is invariant and $m(T) = \mathbf{A}$ on X_n, then $m(\psi(T)) = \psi(\mathbf{A})$ on X_n. The reason for this is that $T|_{X_n}$ and $\mathbf{A}$ have the same eigenvalues. Knowledge of invariant subspaces is equivalent to solving eigenvalue problems. Unfortunately, for practical problems, the analytic eigenvalue problem is intractable. Eigenvalue problems for differential operators are generally solved by constructing a finite difference approximation of the exact differential equation as shown by the following example.

Example 3. Consider the eigenvalue problem for T, i.e.,

$$y'' + \lambda^2 y = 0, \quad y(0) = 0, \quad y(1) = 0.$$

As discussed in the Introduction, a finite difference approximation is

$$\mathbf{AY} = \mu \mathbf{Y}, \quad \mu = h^2 \lambda^2,$$

where $\mathbf{A}$ is defined after Eq. (1.6) and $\mathbf{Y} = (y_1, \cdots, y_{N-1})^T$, $y_i = y(ih)$. The eigenvalues of $\mathbf{A}$ are [9]:

$$\mu_k = 4 \sin^2(\frac{k\pi}{2N}), \quad k = 1, 2, \cdots, N-1,$$

which gives the approximate eigenvalues of T to be

$${}_N\lambda_k^2 = 4N^2 \sin^2(\frac{k\pi}{2N}), \quad k = 1, 2, \cdots, N-1.$$

Clearly $\lim_{N\to\infty}({}_N\lambda_k^2) = k^2\pi^2 = \lambda_k^2$ which are the eigenvalues of T as found in Section 3. Agreement of eigenvalues of T and limiting $\mathbf{A}$ gives us the confidence that the method has merit. In practical situations when N is large (say in hundreds) and k small (say in tens), there is a good agreement between ${}_N\lambda_k^2$ and λ_k^2. This indicates that there is a finite-dimensional invariant subspace X_k spanned by the first k eigenfunctions of T. The restriction of T to X_k, $T|_{X_k}$, is represented by the restriction of $\mathbf{A}$ to $m(X_k)$, the discretized representation of X_k. This implies that the matrix representation of $T^{\frac{\alpha}{2}}|_{X_k}$ is the restriction of $\mathbf{A}^{\frac{\alpha}{2}}$ to $m(X_k)$. Comparison of the analytical solution and the numerical results obtained by this method shows good agreement.

We illustrate the general procedure by the following simple example.

EXAMPLE 4. Use the finite difference method to solve the one dimensional fractional-in-space diffusion equation with initial and boundary-value conditions:

$$\begin{aligned} \frac{\partial\varphi}{\partial t} &= -\kappa(-\triangle)^{\frac{\alpha}{2}}\varphi, \quad 0 < x < 1, && (4.1)\\ \varphi(0,t) &= \varphi(1,t) = 0, && (4.2)\\ \varphi(x,0) &= g(x). && (4.3) \end{aligned}$$

First we apply the finite difference method to the standard BVP:

$$\begin{aligned} \frac{\partial\varphi}{\partial t} &= \kappa\triangle\varphi, \quad 0 < x < 1,\\ \varphi(0,t) &= \varphi(1,t) = 0,\\ \varphi(x,0) &= g(x). \end{aligned}$$

by approximating the space derivatives, but not the time derivative, by a difference expression. The above equations can be written in the following matrix form:

$$\frac{d\mathbf{\Phi}}{dt} = -\eta\mathbf{A}\mathbf{\Phi}, \tag{4.4}$$

where $\eta = \frac{\kappa}{h^2}$ and $\mathbf{A}$ is as given after Eq. (1.6). Assuming that $\frac{1}{h^2}\mathbf{A}$ is a good approximation of the differential operator T, then $m(T^{\frac{\alpha}{2}}) \approx \frac{1}{h^\alpha}\mathbf{A}^{\frac{\alpha}{2}}$ and Eq.(4.1) is approximated by the equation

$$\frac{d\mathbf{\Phi}}{dt} = -\bar{\eta}\mathbf{A}^{\frac{\alpha}{2}}\mathbf{\Phi}, \tag{4.5}$$

where $\bar{\eta} = \frac{\kappa}{h^\alpha}$ and $\mathbf{\Phi}(0)$ is as given in Eq.(1.7). The solution of Eq.(4.5) is given by

$$\mathbf{\Phi}(t) = \exp(-\bar{\eta}\mathbf{A}^{\frac{\alpha}{2}}t)\mathbf{\Phi}(0).$$

For reasonably small values of N, diagonalization is the simplest option for computing the matrix exponential. For $\mathbf{A} \in SPD$, there exits a nonsingular matrix $\mathbf{P} \in \mathbb{R}^{(N-1)\times(N-1)}$ so that

$$\mathbf{A} = \mathbf{P}\mathbf{\Lambda}\mathbf{P}^{\mathbf{T}},$$

where $\mathbf{\Lambda} = diag(\lambda_1, \lambda_2, \cdots, \lambda_{N-1})$ are the eigenvalues of $\mathbf{A}$. The solution of Eq.(4.5) in this case becomes

$$\mathbf{\Phi}(t) = \mathbf{P}\exp(-\bar{\eta}\mathbf{\Lambda}^{\frac{\alpha}{2}}t)\mathbf{P}^T\mathbf{\Phi}(0),$$

where $\exp(-\bar{\eta}\mathbf{\Lambda}^{\frac{\alpha}{2}}t) = diag(\exp(-\bar{\eta}\lambda_1^{\frac{\alpha}{2}}t), \exp(-\bar{\eta}\lambda_2^{\frac{\alpha}{2}}t), \cdots, \exp(-\bar{\eta}\lambda_{N-1}^{\frac{\alpha}{2}}t))$.

Similarly, this technique can be applied to a fractional-in-space diffusion equation with radiating end, or to a multidimensional problem.

Remark 2. Different boundary conditions and/or different discretisation methods may result in matrices $\mathbf{A}$ that are not SPD. In such cases, the matrix function approximation would be more challenging and is a topic for future research.

5. Numerical examples

In this section, we present some numerical results. Numerical solutions are compared with the analytical solution for various boundary conditions.

Example 5. Consider the fractional-in-space diffusion equation

$$\frac{\partial\varphi}{\partial t} = \kappa D_x^\alpha \varphi, \quad 0 < x < \pi, \tag{5.1}$$

$$\varphi(0,t) = \varphi(\pi,t) = 0, \tag{5.2}$$

$$\varphi(x,0) = f(x) = x^2(\pi - x). \tag{5.3}$$

When $\alpha = 2$, $\kappa = 0.25$ and ${}_0D_x^\alpha = {}_0^R D_x^\alpha = -(-\Delta)^{\frac{\alpha}{2}}$, the analytical solution of (5.1)-(5.3) is

$$\varphi(x,t) = \sum_{n=1}^{\infty}\left(\frac{8(-1)^{n+1}-4}{n^3}\right)\sin(nx)\exp(-n^2\kappa t).$$

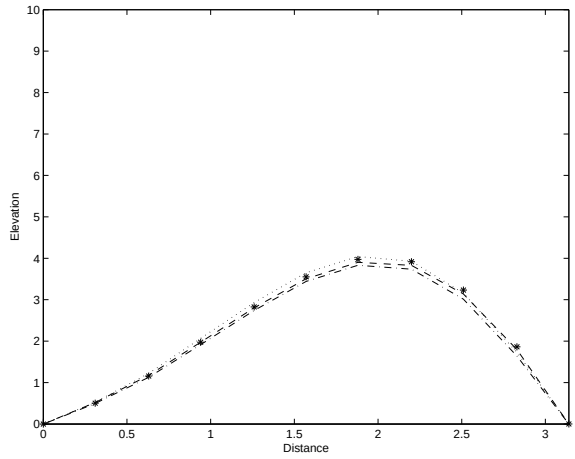

Figure 1: Comparison of the analytical solution $(***)$ and the numerical solutions (matrix method $---$; fractional Caputo $\cdots$; fractional Riesz $-\cdot-\cdot$) at $t = 0.4$ for a fractional-in-space diffusion equation with initial and boundary-value conditions ($\alpha = 1.8$, $\kappa = 0.25$).

When $\alpha \neq 2$, the analytical solution of (5.1)-(5.3) is

$$\varphi(x,t) = \sum_{n=1}^{\infty} \left(\frac{8(-1)^{n+1} - 4}{n^3}\right) \sin(nx) \exp(-(n^2)^{\frac{\alpha}{2}} \kappa t).$$

The analytical solution is compared with the numerical methods in Figure 1 for $t = 0.4$, $\alpha = 1.8$ and $\kappa = 0.25$. It is seen that all three numerical methods perform well, with the matrix method providing the best approximation to the analytical solution.

Example 6. Consider the fractional-in-space diffusion equation with radiating end

$$\frac{\partial \varphi}{\partial t} = -\kappa(-\triangle)^{\frac{\alpha}{2}} \varphi, \quad 0 < x < 1, \tag{5.4}$$

$$\varphi(0,t) = 0, \quad \varphi'(1,t) + \varphi(1,t) = 0, \quad t > 0, \tag{5.5}$$

$$\varphi(x,0) = f(x) = x. \tag{5.6}$$

When $\alpha = 2$ and the analytical solution of (5.4)-(5.6) is

$$\varphi(x,t) = \sum_{n=1}^{\infty} \frac{4\sin(\sqrt{\lambda_n}) \sin(\sqrt{\lambda_n} x)}{\lambda_n (1 + \cos^2 \sqrt{\lambda_n})} \exp(-\lambda_n \kappa t).$$

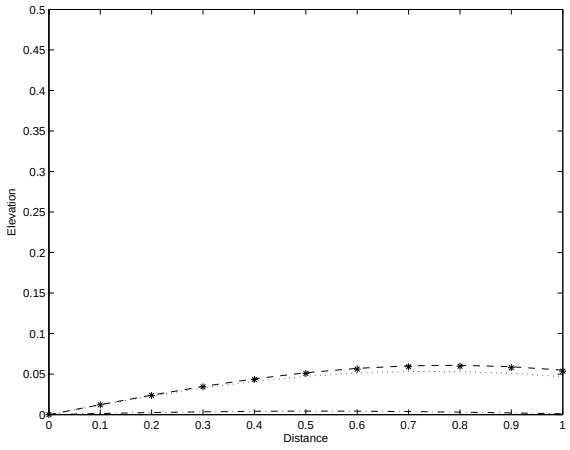

Figure 2: Comparison of the analytical solution ($***$) and the numerical solutions (matrix method $---$; fractional Caputo $\cdots$; fractional Riesz $-\cdot-\cdot$) at $t = 0.7$ for a fractional-in-space diffusion equation with radiating end ($\alpha = 1.8$, $\kappa = 1$).

When $\alpha \neq 2$, the analytical solution of (5.4)-(5.6) is

$$\varphi(x,t) = \sum_{n=1}^{\infty} \frac{4\sin(\sqrt{\lambda_n})\sin(\sqrt{\lambda_n}x)}{\lambda_n(1+\cos^2\sqrt{\lambda_n})} \exp(-\lambda_n^{\frac{\alpha}{2}}\kappa t).$$

The analytical solution and those from the three numerical methods are plotted in Figure 2 for $t = 0.7$, $\alpha = 1.8$ and $\kappa = 1$. The Riesz derivative method performs poorly in this example, while the Caputo derivative method is quite reasonable; but again the matrix method provides the best approximation to the analytical solution.

6. Conclusions

This work has seen a new numerical strategy devised for approximating fractional-in-space diffusion equations. The method is based on solving a system of ordinary differential equations whose matrix $\mathbf{A}$, which represents the spatial discretisation of the Laplacian operator, is raised to a fractional power. The solution of this system presents a matrix function of the form $\exp(-\beta\mathbf{A}^{-\frac{\alpha}{2}})$, $\beta \in \mathbb{R}$, $1 < \alpha < 2$ to be approximated. Although in this work where $\mathbf{A}$ was assumed to be SPD and diagonalisation was used to obtain the desired matrix function, future research will see matrix polynomial

approximations investigated for a wider class of matrices. Finally, a major benefit of this new method is that it can be generalized to higher dimensions without altering the overall solution methodology.

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School of Mathematical Sciences
Queensland University of Technology
GPO Box 2434, Brisbane QLD 4001, AUSTRALIA

e-mails: m.ilic@qut.edu.au , f.liu@qut.edu.au
i.turner@qut.edu.au , v.anh@qut.edu.au

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