

# NUMERICAL APPROXIMATION OF A FRACTIONAL-IN-SPACE DIFFUSION EQUATION (II) – WITH NONHOMOGENEOUS BOUNDARY CONDITIONS \*

# M. Ilic $^1$ , F. Liu $^{1,2}$ , I. Turner $^1$ and V. Anh $^1$

#### Abstract

In this paper, a space fractional diffusion equation (SFDE) with nonhomogeneous boundary conditions on a bounded domain is considered. A new matrix transfer technique (MTT) for solving the SFDE is proposed. 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. Analytic solutions of the SFDE are derived. Finally, some numerical results are given to demonstrate that the MTT is a computationally efficient and accurate method for solving SFDE.

2000 Mathematics Subject Classification: 26A33 (primary), 35S15

Key Words and Phrases: fractional diffusion, anomalous diffusion, nonhomogeneous boundary conditions, numerical approximation

## 1. Introduction

Fractional kinetic equations of the diffusion and Fokker-Planck type have been proposed as a useful approach for the description of transport dynamics in complex systems that are governed by anomalous diffusion and non-exponential relaxation patterns [19].

<sup>\*</sup> This research was partially supported by the Australian Research Council, Grant LP0348653 and the National Natural Science Foundation of China, Grant 10271098

Space fractional diffusion equations have been investigated by West and Seshadri [23] and more recently by Gorenflo and Mainardi [7, 8]. However numerical methods for these fractional equations are still under development. Some different numerical methods for solving fractional partial differential equations have been proposed. Liu et al. [14, 15, 16] transformed a fractional partial differential equation into a system of ordinary differential equations using the fractional method of Lines, which was then solved using backward differentiation formulas. Meerschaert et al. [18] proposed finite difference approximations for fractional-in-space advection-dispersion flow equations.

Part I of the present study explored the possibility of representing the fractional Laplacian  $(-\Delta)^{\frac{\alpha}{2}}$  in one-dimensional space subject to homogeneous boundary conditions in matrix form  $\mathbf{A}^{\frac{\alpha}{2}}$ . Here the entries of  $\mathbf{A}$  were generated using finite difference approximations. Spectral decomposition played the central role in our understanding of this representation. The key result is summarized by the following definition:

DEFINITION 1. Suppose the Laplacian  $(-\triangle)$  has a complete set of orthonormal eigenfunctions  $\varphi_n$  corresponding to eigenvalues  $\lambda_n^2$  on a bounded region  $\mathcal{D}$  i.e.  $(-\triangle)\varphi_n = \lambda_n^2 \varphi_n$  on  $\mathcal{D}$ ;  $\mathcal{B}(\varphi) = 0$  on  $\partial \mathcal{D}$ , where  $\mathcal{B}(\varphi)$  is one of the standard three homogeneous boundary conditions. Let

$$\mathcal{F}_{\gamma} = \{ f = \sum_{n=1}^{\infty} c_n \varphi_n, \quad c_n = \langle f, \varphi_n \rangle | \sum_{n=1}^{\infty} |c_n|^2 |\lambda|_n^{\gamma} < \infty, \quad \gamma = \max(\alpha, 0) \}$$
  
Then for any  $f \in \mathcal{F}_{\gamma}, \ (-\Delta)^{\frac{\alpha}{2}}$  is defined by

Then for any  $f \in \mathcal{F}_{\gamma}, (-\triangle)^{\frac{\alpha}{2}}$  is defined by

$$(-\triangle)^{\frac{\alpha}{2}}f = \sum_{n=1} c_n \lambda_n^{\alpha} \varphi_n.$$

REMARK 1. The operator  $T = (-\Delta)^{\frac{\alpha}{2}}$  is linear and self-adjoint, i.e., if  $f = \sum_{n=1}^{\infty} a_n \varphi_n$  and  $g = \sum_{n=1}^{\infty} b_n \varphi_n$ , then  $\langle Tf, g \rangle = \sum_{n=1}^{\infty} a_n b_n \lambda_n^{\alpha} \varphi_n = \langle f, Tg \rangle$ .

REMARK 2. If 
$$f \in \mathcal{F}_{\gamma}$$
 where  $\gamma = \max(0, \alpha, \beta, \alpha + \beta)$ , then  
 $(-\Delta)^{\frac{\alpha}{2}}(-\Delta)^{\frac{\beta}{2}}f = (-\Delta)^{\frac{\alpha}{2}}\left\{\sum_{n=1}^{\infty}c_n\lambda_n^{\beta}\varphi_n\right\}$   
 $= \sum_{n=1}^{\infty}c_n\lambda_n^{\alpha+\beta}\varphi_n = (-\Delta)^{\frac{\alpha+\beta}{2}}f = (-\Delta)^{\frac{\beta}{2}}(-\Delta)^{\frac{\alpha}{2}}f$ 

REMARK 3. For  $\alpha < 0$ , the only problem that can arise is if  $\lambda = 0$  is an eigenvalue. As for ordinary Laplacian, care is required in this case, or

one can use the Bessel operator  $(I - \Delta)^{\frac{\alpha}{2}}$ , which is the inverse of the Bessel potential  $(I - \Delta)^{-\frac{\alpha}{2}}$ ,  $\alpha \in \mathbb{R}_+$ , defined by the kernel

$$I_{\alpha}(x) = \frac{1}{(4\pi)^{\alpha/2}} \frac{1}{\Gamma(\alpha/2)} \int_{0}^{\infty} e^{-\pi|x|^{2}/s} e^{-s/4\pi} s^{(-n+\alpha)/2} \frac{ds}{s}, \quad x \in \mathbb{R}.$$

It is known that  $I_{\alpha}(x) \in L^{1}(\mathbb{R})$  and its Fourier transform is

$$\hat{I}_{\alpha}(\lambda) = (2\pi)^{-1/2}(1+|\lambda|^2) - \alpha/2, \lambda \in \mathbb{R}.$$

REMARK 4. For  $\alpha > 0$ , Definition 1 may be too restrictive, since ordinary functions (and in particular solutions of partial differential equations) may not belong to  $\mathcal{F}_{\alpha}$ . The resulting series may not converge, or not converge uniformly.

REMARK 5. It is reasonable to expect that if  $f \in \mathcal{F}_{\alpha}$ , then f = 0 on  $\partial \mathcal{D}$ . The question arises what is the effect of  $(-\Delta)^{\frac{\alpha}{2}}$  on a function which does not satisfy the homogeneous boundary conditions. Put another way, how does one solve problems with nonhomogeneous boundary conditions? According to Podlubny [20], even the form of boundary conditions has not been completely defined for fractional derivatives.

In Section 2 we propose an extension to Definition 1 to overcome the problems mentioned in Remarks 4 and 5.

In this paper, the following space fractional diffusion equation (SFDE) with initial and nonhomogeneous boundary-value conditions in 1-D is considered.

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

$$\frac{\partial \varphi}{\partial t} = -\kappa \left( -\frac{\partial^2}{\partial x^2} \right)^{\frac{\alpha}{2}} \varphi, \quad 0 < x < L, \tag{1.1}$$

with the initial condition

$$\varphi(x,0) = F(x) \tag{1.2}$$

together with one of the following boundary conditions:

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

This paper is organized as follows: Section 3 proposes a new matrix transfer technique (MTT) for the SFDE; Section 4 derives the analytic solution of the SFDE. Finally, we present some numerical results to demonstrate that the MTT is computationally straightforward for the SFDE.

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

#### 2. Fractional operator and its extension

First we wish to extend the Definition 1 for any  $\alpha$  and all sufficiently differentiable functions. Consider the expansion  $f = \sum_{n=1}^{\infty} c_n \varphi_n$  as discussed in Definition 1. Although it may not be true that  $(-\Delta)f = \sum_{n=1}^{\infty} c_n(-\Delta)\varphi_n$  $= \sum_{n=1}^{\infty} c_n \lambda_n^2 \varphi_n$ , it is reasonable to expect that if  $g = (-\Delta)f = -f_{xx}$ ; (for example), then under mild conditions we can write  $g = \sum_{n=1}^{\infty} b_n \varphi_n$ . This idea is captured in the following definition:

DEFINITION 2. Let  $\{\varphi_n\}$  be a complete set of orthonormal eigenfunctions corresponding to eigenvalues  $\lambda_n^2$  of the Laplacian  $(-\Delta)$  on a bounded region  $\mathcal{D}$  with homogeneous boundary conditions on  $\mathcal{D}$ . Then

$$(-\triangle)^{\frac{\alpha}{2}}f = \begin{cases} (-\triangle)^m f & \text{if } \alpha = 2m, \ m = 0, 1, 2...\\ (-\triangle)^{\frac{\alpha}{2}-m}(-\triangle)^m f & \text{if } m - 1 < \frac{\alpha}{2} < m, \ m = 1, 2, ...\\ \sum_{n=1}^{\infty} \lambda_n^{\alpha} \langle f, \varphi_n \rangle \varphi_n & \text{if } \alpha < 0 \end{cases}$$

REMARK 6. Clearly, this is in the spirit of Definition 1 and is analogous to the Caputo definition. If  $f \in \mathcal{F}_{\gamma}$ ,  $\gamma = \alpha > 0$  as in Remark 2 after Definition 1, then there is no need to split the exponent as indicated in the second line above; the two definitions are identical.

Next consider the extension of the action of  $(-\triangle)^{\frac{\alpha}{2}}$  on functions which do not satisfy homogeneous boundary conditions. To accomplish this task, we derive an expression which is analogous to the classical Green's formula. Although the method can be extended to two or three dimensions we consider only the one dimensional case in this paper. We also restrict  $\alpha$  to satisfy  $0 < \alpha \leq 2$  which is relevant in practice.

PROPOSITION 1. Let  $\varphi_n(x)$  be an eigenfunction corresponding to the eigenvalue  $\lambda_n^2$  of the Laplacian  $(-\triangle) = (-\frac{d^2}{dx^2})$  on the interval  $a \leq x \leq b$ , and f any sufficiently smooth function. Then

$$\langle \varphi_n, (-\Delta)^{\frac{\alpha}{2}} f \rangle - \langle (-\Delta)^{\frac{\alpha}{2}} \varphi_n, f \rangle$$
  
=  $\lambda_n^{\alpha-2} [f(b)\varphi'_n(b) - f(a)\varphi'_n(a) - f'(b)\varphi_n(b) + f'(a)\varphi_n(a)]$ 

P r o o f. From Definition 2 and  $0 < \alpha < 2, m = 1$ ,

$$\langle \varphi_n, (-\Delta)^{\frac{\alpha}{2}} f \rangle = \langle \varphi_n, (-\Delta)^{\frac{\alpha}{2}-1} (-\Delta) f \rangle$$

$$= \langle (-\Delta)^{\frac{\alpha}{2}-1} \varphi_n, (-\Delta) f \rangle$$

$$= \lambda_n^{\alpha-2} \langle \varphi_n, -f_{xx} \rangle = \lambda_n^{\alpha-2} \int_a^b \varphi_n (-f_{xx}) \, dx$$

$$(2.1)$$

$$= \lambda_n^{\alpha-2} [f(b)\varphi'_n(b) - f(a)\varphi'_n(a) - f'(b)\varphi_n(b) + f'(a)\varphi_n(a) - \int_a^b \varphi''_n f \, dx] = \lambda_n^{\alpha} \langle \varphi_n, f \rangle + \lambda_n^{\alpha-2} [f(b)\varphi'_n(b) - f(a)\varphi'_n(a) - f'(b)\varphi_n(b) + f'(a)\varphi_n(a)] = \langle (-\Delta)^{\frac{\alpha}{2}}\varphi_n, f \rangle + \lambda_n^{\alpha-2} [f(b)\varphi'_n(b) - f(a)\varphi'_n(a) - f'(b)\varphi_n(b) + f'(a)\varphi_n(a)],$$

using integration by parts and self-adjointness of  $(-\triangle)^{\frac{\alpha}{2}-1}$ .

#### 

#### 3. Matrix Transfer Technique for the SFDE

In this section, a new matrix transfer technique for the SFDE is proposed. The method will be illustrated by two examples; the first involves Dirichlet type boundary conditions, while the second involves a boundary condition of the third type.

EXAMPLE 1. Use the finite difference method to solve the one-dimensional fractional-in-space diffusion equation with initial and boundary-value conditions given as follows:

$$\frac{\partial \varphi}{\partial t} = -k(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}\varphi, \quad 0 < x < 1, \ t > 0, \tag{3.1}$$

$$\varphi(0,t) = f(t), \quad t > 0,$$
 (3.2)

$$\varphi(1,t) = g(t), t > 0,$$
 (3.3)

$$\varphi(x,0) = F(x), \quad 0 < x < 1.$$
 (3.4)

First, the standard space diffusion equation with initial boundary-value conditions is considered:

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

$$\varphi(0,t) = f(t), \quad t > 0,$$
(3.6)

$$\varphi(1,t) = g(t), \quad t > 0,$$
 (3.7)

$$\varphi(x,0) = F(x), \quad 0 < x < 1. \tag{3.8}$$

Secondly, we introduce a finite difference approximation for the spatial derivative:

$$\frac{d\varphi_i}{dt} = -\frac{k}{h^2}(-\varphi_{i+1} + 2\varphi_i - \varphi_{i-1}), \quad (i = 1, \cdots, N-1), \quad (3.9)$$

$$\varphi_0 = f(t), \qquad (3.10)$$

$$\varphi_N = g(t), \tag{3.11}$$

$$\varphi(x_i, 0) = F(x_i), \quad (i = 1, \cdots, N-1).$$
 (3.12)

where  $\varphi_i = \varphi(x_i, t)$ , h is the discrete spatial step and  $N = \frac{1}{h}$ .

The above equations can be rewritten in the following matrix form:

$$\frac{\mathbf{d\Phi}}{\mathbf{dt}} = -k(\mathbf{A\Phi} - \frac{1}{h^2}\mathbf{e}_1 f(t) - \frac{1}{h^2}\mathbf{e}_{N-1}g(t)), \qquad (3.13)$$

where  $\mathbf{A} = \frac{1}{h^2} tridiag(-1, 2, -1)$ , and  $\mathbf{e}_1$ ,  $\mathbf{e}_{N-1}$  are the  $1^{st}$  and  $(N-1)^{th}$  canonical basis vectors in  $\mathbb{R}^{N-1}$ .

For a real nonsingular, symmetric matrix  $\mathbf{A}_{(N-1)\times(N-1)}$ , there exits a nonsingular matrix  $\mathbf{P}_{(N-1)\times(N-1)}$  such that

$$\mathbf{A} = \mathbf{P} \mathbf{\Lambda} \mathbf{P}^{\mathbf{T}} \tag{3.14}$$

where  $\Lambda = diag(\lambda_1, \lambda_2, \dots, \lambda_{N-1})$  and  $\lambda_i (i = 1, 2, \dots, N-1)$  are the eigenvalues of **A**.

Thirdly, we consider the equation (3.1) rewritten in the following form:

$$\frac{\partial \varphi}{\partial t} = -k(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}-1}(-\frac{\partial^2}{\partial x^2})\varphi.$$

Let  $\mathbf{A} = \mathbf{m}(-\frac{\partial^2}{\partial x^2})$  be the matrix representation of the Laplacian, where we impose homogeneous boundary conditions. If the function  $\varphi$  does not satisfy the homogeneous boundary conditions, then

$$\mathbf{m}(-\frac{\partial^2\varphi}{\partial x^2}) = \mathbf{A}\mathbf{\Phi} - \frac{1}{h^2}\mathbf{e}_1 f(t) - \frac{1}{h^2}\mathbf{e}_{N-1}g(t).$$

Now a space fractional diffusion equation (3.1) with initial and nonhomogeneous boundary-value conditions (3.2-3.4) in one-dimension is considered. Assuming the fractional Laplacian satisfies  $\mathbf{m}\left\{\left(-\frac{\partial^2}{\partial x^2}\right)^{\frac{\alpha}{2}-1}\right\} = \mathbf{A}^{\frac{\alpha}{2}-1}$ , the equations (3.1) with (3.2-3.3) can be rewritten as follows:

$$\frac{\mathbf{d\Phi}}{\mathbf{dt}} = -k\mathbf{A}^{\frac{\alpha}{2}-1}(\mathbf{A\Phi} - \frac{1}{h^2}\mathbf{e}_1f(t) - \frac{1}{h^2}\mathbf{e}_{N-1}g(t)) \qquad (3.15)$$
$$= -k\mathbf{A}^{\frac{\alpha}{2}}\mathbf{\Phi} + \frac{k}{h^2}\mathbf{A}^{\frac{\alpha}{2}-1}\mathbf{e}_1f(t) + \frac{k}{h^2}\mathbf{A}^{\frac{\alpha}{2}-1}\mathbf{e}_{N-1}g(t).$$

EXAMPLE 2. Solve the following one dimensional fractional-in-space diffusion equation with a radiating end:

$$\frac{\partial \varphi}{\partial t} = -k(-\Delta)^{\frac{\alpha}{2}}\varphi, \quad 0 < x < 1, \tag{3.16}$$

$$\varphi(0,t) = f(t), \quad \varphi'(1,t) + \varphi(1,t) = g(t), \quad t > 0,$$
 (3.17)

$$\varphi(x,0) = F(x). \tag{3.18}$$

The procedure followed in Example 1 again applies. The only difference is that one additional finite difference equation needs to be added for the boundary value  $\varphi_N$  so that for this example **A** is  $N \times N$ . This is explained further as follows.

From (3.9), when i = N we have  $d\varphi_N \qquad k$ 

$$\frac{d\varphi_N}{dt} \approx \frac{k}{h^2} \{\varphi_{N+1} - 2\varphi_N + \varphi_{N-1}\},\tag{3.19}$$

and Eq. (3.17) becomes

$$\frac{\varphi_{N+1} - \varphi_N}{h} + \varphi_N = g(t), \qquad (3.20)$$

or, rearranging

$$\varphi_{N+1} = hg(t) + (1-h)\varphi_N.$$
 (3.21)

Eq. (3.19) becomes

$$\frac{d\varphi_N}{dt} \approx \frac{k}{h^2} \{hg(t) - h\varphi_N + \varphi_{N-1} - \varphi_N\}$$

$$= -\frac{k}{h^2} \{(1+h)\varphi_N - \varphi_{N-1}\} + \frac{k}{h}g(t).$$
(3.22)

From Eq. (3.22), the last row of matrix  $\mathbf{A}_{N \times N}$  is then given by

$$\frac{1}{h^2}(\mathbf{0}_{1\times N-2} - 1 \ (1+h)).$$

In order to solve ODE systems of the form (3.15) we inject the spectral decomposition of **A**, to arrive at the method we call the matrix transfer technique (MTT).

Thus, for Example 2,

$$\frac{\mathbf{d}\Phi}{\mathbf{d}\mathbf{t}} = -k\mathbf{P}\mathbf{\Lambda}^{\frac{\alpha}{2}}\mathbf{P}^{\mathbf{T}}\Phi + \frac{k}{h^{2}}\mathbf{P}\mathbf{\Lambda}^{\frac{\alpha}{2}-1}\mathbf{P}^{\mathbf{T}}\mathbf{e}_{1}f(t) + \frac{k}{h}\mathbf{P}\mathbf{\Lambda}^{\frac{\alpha}{2}-1}\mathbf{P}^{\mathbf{T}}\mathbf{e}_{N}g(t), \quad (3.23)$$
  
where  $\Lambda^{\frac{\alpha}{2}} = diag(\lambda_{1}^{\frac{\alpha}{2}}, \lambda_{2}^{\frac{\alpha}{2}}, \cdots, \lambda_{N}^{\frac{\alpha}{2}}).$ 

In this work, we can use the differential/algebraic system solver (DASSL) [5] as our ODE solver. DASSL approximates the time derivative using the k-th order BDF, where k ranges from order one to five. At every step, it chooses the order k and step size based on the behaviour of the solution. This technique has been used to solve adsorption problems involving step gradients in bidisperse solids [10, 13], hyperbolic models of transport in bidisperse solids [11], transport problems involving steep concentration gradients [12], modelling saltwater intrusion into coastal aquifers [14, 17], numerical simulation for the space fractional Fokker-Planck equation [15, 16] and the space fractional diffusion equation with insulated ends [21].

#### 4. Analytic solution of the SFDE

In order to demonstrate that the MTT is effective in obtaining an approximate solution of the SFDE, the computed solution will be compared with the analytic solution of the SFDE, which will be derived in this section. Again we consider the two examples presented in the previous section.

EXAMPLE 3. Obtain the analytic solution of the SFDE (3.1-3.4).

With  $\langle f,g\rangle = \int_0^1 f(x)g(x)dx$  as the inner product, the operator  $-\frac{\partial^2}{\partial x^2}$ ,  $\varphi(0) = \varphi(1) = 0$  is self-adjoint and has eigenfunctions  $\varphi_n(x) = \sqrt{2}\sin(n\pi x)$  and corresponding eigenvalues  $\lambda_n^2 = (n\pi)^2$ ,  $n = 1, 2, \ldots$  The operator  $(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}$  as a function of  $(-\frac{\partial^2}{\partial x^2})$  is also self-adjoint. We can extend its definition to functions that do not vanish at x = 0 and x = 1 as follows:

$$\begin{aligned} \langle \varphi_n, (-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}} \varphi \rangle &= \langle \varphi_n, (-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}-1} (-\frac{\partial^2}{\partial x^2} \varphi) \rangle \end{aligned} \tag{4.1} \\ &= \langle (-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}-1} \varphi_n, (-\frac{\partial^2}{\partial x^2}) \varphi \rangle = \lambda_n^{\alpha-2} \langle \varphi_n, -\varphi'' \rangle \\ &= \lambda^{\alpha} \langle \varphi_n, \varphi \rangle + \lambda_n^{\alpha-2} [\varphi(1) \varphi'_n(1) - \varphi(0) \varphi'_n(0)] \end{aligned}$$

using integration by parts.

To derive the analytic solution of the SFDE, we apply the Laplace transform method to equations (3.1-3.3) as follows:

$$s\overline{\varphi} - F = -k(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}\overline{\varphi}(x,s), \qquad (4.2)$$

$$\overline{\varphi}(0,s) = f(s), \tag{4.3}$$

$$\overline{\varphi}(1,s) = \overline{g}(s), \tag{4.4}$$

where  $\overline{\varphi}(x,s) = L\varphi(x,t) = \int_0^\infty e^{-st}\varphi(x,t)dt$  is the Laplace transform of  $\varphi(x,t)$ .

Taking the finite transform with respect to  $\{\varphi_n(x)\}$ , the eigenfunctions generated by  $(-\frac{\partial^2}{\partial x^2})$  with homogeneous boundary conditions, we obtain  $\varphi_n(x) = \sqrt{2}\sin(n\pi x), \ \varphi'_n(x) = \sqrt{2}n\pi\cos(n\pi x)$ . Thus,  $\varphi'_n(1) = \sqrt{2}n\pi(-1)^n$  and  $\varphi'_n(0) = \sqrt{2}n\pi, \ \lambda_n = n\pi$ .

$$s\langle\varphi_n,\overline{\varphi}(x,s)\rangle - \langle\varphi_n,F\rangle = -k\langle\varphi_n,(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}\overline{\varphi}\rangle$$

$$= -k\langle(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}\varphi_n,\overline{\varphi}\rangle - k\lambda_n^{\alpha-2}[\overline{g}(s)\varphi_n'(1) - \overline{f}(s)\varphi_n'(0)].$$
(4.5)

Set  $\langle \varphi_n, \overline{\varphi}(x,s) \rangle = C_n(s), \langle \varphi_n, F \rangle = F_n$ , we have

$$(k\lambda_n^{\alpha} + s)C_n(s) = F_n - k\lambda_n^{\alpha-2}[\overline{g}(s)\varphi'_n(1) - \overline{f}(s)\varphi'_n(0)].$$

$$C_n(s) = \frac{F_n}{k\lambda_n^{\alpha} + s} - \frac{k\lambda_n^{\alpha-2}}{k\lambda_n^{\alpha} + s}[\overline{g}(s)\varphi'_n(1) - \overline{f}(s)\varphi'_n(0)] \qquad (4.6)$$

$$= \frac{F_n}{k\lambda_n^{\alpha} + s} + \frac{\sqrt{2}}{\lambda_n}(-1)^{n+1}\overline{g}(s)$$

$$+ \frac{\sqrt{2}}{\lambda_n}\overline{f}(s) + \frac{\sqrt{2}s}{\lambda_n(k\lambda_n^{\alpha} + s)}\{\overline{g}(s)(-1)^n - \overline{f}(s)\},$$

where the splitting in the second line was done to improve the convergence of the sum in (4.7).

Hence,

$$\overline{\varphi}(x,s) = \sum_{n=1}^{\infty} C_n(s)\varphi_n(x)$$

$$= \sum_{n=1}^{\infty} \frac{\sqrt{2F_n}}{k\lambda_n^{\alpha} + s} \sin(n\pi x) + x\overline{g}(s) + (1-x)\overline{f}(s)$$

$$+ 2\sum_{n=1}^{\infty} \frac{1}{\lambda_n(k\lambda_n^{\alpha} + s)} \{s\overline{g}(s)(-1)^n - s\overline{f}(s)\} \sin(n\pi x).$$

$$(4.7)$$

In general,

$$\varphi(x,t) = \sum_{n=1}^{\infty} \sqrt{2} F_n e^{-k\lambda_n^{\alpha} t} \sin(n\pi x) + xg(t) + (1-x)f(t) \qquad (4.8)$$
$$+ 2\sum_{n=1}^{\infty} \frac{\sin(n\pi x)}{\lambda_n} \int_0^t e^{-k\lambda_n^{\alpha}(t-\tau)} \{(-1)^n G(\tau) - h(\tau)\} d\tau$$

with  $L^{-1}\{s\overline{g}(s)\} = G(t)$  and  $L^{-1}\{s\overline{f}(s)\} = h(t)$ .

In our numerical example, we take  $f(t) = g(t) = e^{-t}$  and  $F(x) = -(x^2 - x - 1)$ . Thus,  $\overline{g}(s) = \overline{f}(s) = \frac{1}{s+1}$ .

Using partial fractions

$$\frac{s}{(k\lambda_n^{\alpha}+s)(s+1)} = \frac{A}{k\lambda_n^{\alpha}+s} + \frac{B}{s+1},$$

where  $A = \frac{k\lambda_n^{\alpha}}{k\lambda_n^{\alpha-1}}$ ,  $B = -\frac{1}{k\lambda_n^{\alpha-1}}$ . Noting that  $L^{-1}\left\{\frac{1}{s+a}\right\} = e^{-at}$ , we obtain

$$\varphi(x,t) = \sum_{n=1}^{\infty} \sqrt{2} F_n e^{-k\lambda_n^{\alpha} t} \sin(n\pi x) + xg(t) + (1-x)f(t) \quad (4.9)$$
  
+ 
$$2\sum_{n=1}^{\infty} \frac{\{(-1)^n - 1\}}{\lambda_n} \frac{k\lambda_n^{\alpha}}{k\lambda_n^{\alpha} - 1} e^{-k\lambda_n^{\alpha} t} \sin(n\pi x)$$
  
- 
$$2\sum_{n=1}^{\infty} \frac{\{(-1)^n - 1\}}{\lambda_n} \frac{\sin(n\pi x)}{k\lambda_n^{\alpha} - 1} e^{-t},$$

where

$$F_n = \langle \varphi_n, F \rangle = -\sqrt{2} \{ \frac{2}{(n\pi)^3} + \frac{1}{n\pi} \} [(-1)^n - 1].$$
 (4.10)

Therefore, we obtain the solution of (3.1-3.4) for this choice of f(t) and g(t) as:

$$\varphi(x,t) = -\sum_{n=1}^{\infty} 2\sin(n\pi x) \{\frac{2}{(n\pi)^3} + \frac{1}{n\pi}\} [(-1)^n - 1] e^{-k(n\pi)^{\alpha}t}$$
(4.11)

$$+xe^{-t} + (1-x)e^{-t} + 2\sum_{n=1}^{\infty} \frac{\{(-1)^n - 1\}k(n\pi)^{\alpha-1}}{k(n\pi)^{\alpha} - 1}e^{-k(n\pi)^{\alpha}t}\sin(n\pi x)$$
$$-2\sum_{n=1}^{\infty} \frac{\{(-1)^n - 1\}}{n\pi}\frac{\sin(n\pi x)}{k(n\pi)^{\alpha} - 1}e^{-t}.$$

EXAMPLE 4. Obtain the analytic solution of the SFDE (3.16-3.18).

The eigenvalues  $\{\lambda_n^2\}$  and eigenfunctions  $\{\varphi_n\}$  are obtained as in Example 2 in Part 1 of the paper [9]. The eigenvalues  $\{\lambda_n^2\}$  must satisfy

$$\sin(\lambda x) + \lambda \cos(\lambda x) = 0.$$

The corresponding normalized eigenfunctions are

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

The analytic solution is derived by the transform method as outlined in the previous example.

Application of the Laplace transform gives

$$s\overline{\varphi} - F = -k(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}\overline{\varphi}(x,s), \qquad (4.12)$$
$$\overline{\psi}(0,s) = \overline{\psi}(s) \qquad (4.12)$$

$$\overline{\varphi}(0,s) = f(s), \tag{4.13}$$

$$\overline{\varphi}'(1,s) + \overline{\varphi}(1,s) = \overline{g}(s). \tag{4.14}$$

Applying the finite transform with respect to  $\{\varphi_n(x)\}$  gives

$$s\langle\varphi_{n},\overline{\varphi}(x,s)\rangle - \langle\varphi_{n},F\rangle$$

$$= -k\lambda_{n}^{\alpha}\langle\varphi_{n},\overline{\varphi}(x,s)\rangle + k\lambda_{n}^{\alpha-2}\frac{\sqrt{2}}{\sqrt{1+\cos^{2}\lambda_{n}}}[\overline{g}(s)\sin\lambda_{n} + \lambda_{n}\overline{f}(s)]$$

$$(4.15)$$

From (4.15) and set  $C_n = \langle \varphi_n, \overline{\varphi}(x, s) \rangle$  to obtain:

$$C_{n} = \frac{F_{n}}{k\lambda_{n}^{\alpha} + s} + \frac{k\lambda_{n}^{\alpha-2}\sqrt{2}\overline{g}\sin\lambda_{n}}{(s+k\lambda_{n}^{\alpha})\sqrt{1+\cos^{2}\lambda_{n}}} + \frac{k\sqrt{2}\lambda_{n}^{\alpha-1}\overline{f}}{(s+k\lambda_{n}^{\alpha})\sqrt{1+\cos^{2}\lambda_{n}}} = \frac{F_{n}}{k\lambda_{n}^{\alpha} + s} + \frac{\overline{g}}{2}\frac{2\sqrt{2}\sin\lambda_{n}}{\lambda_{n}^{2}\sqrt{1+\cos^{2}\lambda_{n}}}(1-\frac{s}{s+k\lambda_{n}^{\alpha}}) + \frac{\overline{f}\sqrt{2}}{\lambda_{n}\sqrt{1+\cos^{2}\lambda_{n}}}(1-\frac{s}{s+k\lambda_{n}^{\alpha}}) = \frac{F_{n}}{k\lambda_{n}^{\alpha} + s} + \frac{\overline{g}}{2}\frac{2\sqrt{2}\sin\lambda_{n}}{\lambda_{n}^{2}\sqrt{1+\cos^{2}\lambda_{n}}} - \frac{\overline{g}}{2}\frac{s2\sqrt{2}\sin\lambda_{n}}{\lambda_{n}^{2}\sqrt{1+\cos^{2}\lambda_{n}}}(s+k\lambda_{n}^{\alpha}) + \frac{\overline{f}\sqrt{2}}{\lambda_{n}\sqrt{1+\cos^{2}\lambda_{n}}} - \frac{\overline{f}\sqrt{2}s}{\lambda_{n}\sqrt{1+\cos^{2}\lambda_{n}}}(s+k\lambda_{n}^{\alpha}).$$
(4.16)

where the splitting was again used to improve convergence. Hence,

$$\overline{\varphi}(x,s) = \sum_{n=1}^{\infty} C_n(s)\varphi_n(x) \qquad (4.17)$$

$$= \sum_{n=1}^{\infty} \frac{F_n}{k\lambda_n^{\alpha} + s}\varphi_n(x) + \frac{\overline{g}}{2}x + \overline{f}(1 - \frac{x}{2})$$

$$-\overline{g}\sqrt{2}s\sum_{n=1}^{\infty} \frac{\sin\lambda_n\varphi_n(x)}{\lambda_n^2\sqrt{1 + \cos^2\lambda_n}(s + k\lambda_n^{\alpha})}$$

$$-\overline{f}\sqrt{2}s\sum_{n=1}^{\infty} \frac{\varphi_n(x)}{\lambda_n\sqrt{1 + \cos^2\lambda_n}(s + k\lambda_n^{\alpha})}.$$

In our numerical example, we take  $f(t) = g(t) = e^{-t}$  and  $F(x) = -(x^2 - x - 1)$ . Thus, we have

$$F_{n} = -\int_{0}^{1} (x^{2} - x - 1) \frac{\sqrt{2} \sin(\lambda_{n} x)}{\sqrt{1 + \cos^{2}(\lambda_{n})}}$$
(4.18)  
$$= \frac{\sqrt{2}}{\lambda_{n} \sqrt{1 + \cos^{2}(\lambda_{n})}} - \frac{2\sqrt{2} (\cos \lambda_{n} - 1)}{\lambda_{n}^{3} \sqrt{1 + \cos^{2}(\lambda_{n})}}.$$

Therefore, we obtain

$$\varphi(x,t) = \sqrt{2} \sum_{n=1}^{\infty} \frac{F_n \sin(\lambda_n x)}{\sqrt{1 + \cos^2 \lambda_n}} e^{-k\lambda_n^{\alpha} t} + \frac{x}{2}g(t) + (1 - \frac{x}{2})f(t) \quad (4.19)$$
$$- 2\sum_{n=1}^{\infty} \frac{\sin(\lambda_n x)(\sin \lambda_n + \lambda_n)}{\lambda_n^2 (k\lambda_n^{\alpha} - 1)\sqrt{1 + \cos^2 \lambda_n}} \{k\lambda_n^{\alpha} e^{-k\lambda_n^{\alpha} t} - e^{-t}\}.$$

### 5. Numerical examples

In this section, we present some numerical results. Numerical solutions are compared with the analytic solutions.

EXAMPLE 5. Fractional in space diffusion equation in 1-D:

$$\frac{\partial \varphi}{\partial t} = -k(-\frac{\partial^2}{\partial x^2})^{\frac{\alpha}{2}}\varphi, \quad 0 < x < 1, \ t > 0, \tag{5.1}$$

$$\varphi(0,t) = f(t), t > 0,$$
 (5.2)

$$\varphi(1,t) = g(t), \quad t > 0,$$
 (5.3)

$$\varphi(x,0) = F(x), \quad 0 < x < 1,$$
(5.4)

where k = 0.5,  $f(t) = e^{-t}$ ,  $g(t) = e^{-t}$ ,  $F(x) = -(x^2 - x - 1)$ .

Figure 1 shows the effect of fractional order  $\alpha$ , while Figure 2 shows the effect of time t. From these figures, it can be seen that the numerical solution (MTT) is in good agreement with the analytic solution.

EXAMPLE 6. Fractional-in-space diffusion equation with radiating end  $(BC)_3$  in one dimension:

$$\frac{\partial \varphi}{\partial t} = -\kappa (-\Delta)^{\frac{\alpha}{2}} \varphi, \quad 0 < x < 1, \tag{5.5}$$

$$\varphi(0,t) = f(t), \quad \varphi'(1,t) + \varphi(1,t) = g(t), \quad t > 0, \tag{5.6}$$

$$\varphi(x,0) = F(x), \tag{5.7}$$

where k = 0.5,  $f(t) = e^{-t}$ ,  $g(t) = e^{-t}$ ,  $F(x) = -(x^2 - x - 1)$ .



Figure 1: Comparison of numerical solution (curves) and analytic solution (symbols) at t = 1 for a space fractional diffusion equation with  $\kappa = 0.5$  and  $\alpha = 1.5, 1.6, 1.7, 1.8, 1.9$ , respectively.

Figures 3 and 4 show the effect of time t for a space fractional diffusion equation with a radiating end  $(BC)_3$ , and with  $\alpha = 1.9$  and  $\alpha = 1.8$ respectively. From these figures, it can be seen that the numerical solution (MTT) is in good agreement with the analytic solution.

#### 6. Conclusions

In this paper a novel numerical solution technique for solving SFDE with nonhomogeneous boundary conditions of Type I and Type III has been derived. The innovation of the MTT method is that it leads to a system of ODEs with spatial discretisation matrix raised to the fractional order. Comparisons with two analytical solutions highlight that MTT provides an accurate simulation of the fractional-in-space diffusion equations.

#### References

 E.J. Allen, J. Baglama, and S.K. Boyd, Numerical approximation of the product of the square root of a matrix with a vector. *Linear Algebra Appl.* **310** (2000), 167-181.



Figure 2: Comparison of numerical solution (curves) and analytic solution (symbols) for a space fractional diffusion equation with  $\kappa = 0.5$ ,  $\alpha = 1.8$ , and at t = 0.1, 0.3, 0.5, 0.7, 0.9, respectively.

- [2] V.V. Anh and N.N. Leonenko, Spectral analysis of fractional kinetic equations with random data. J. Statistical Physics 104 (2001), 239-252.
- [3] V.V. Anh and N.N. Leonenko, Renormalization and homogenization of fractional diffusion equations with random data. *Probability Theory* and Related Fields 124 (2002), 381-408.
- [4] V.V. Anh and N. N. Leonenko, Harmonic analysis of random fractional diffusion-wave equations. *Journal of Applied Mathematics and Computation* 141 (2003), 77-85.
- [5] K.E. Brenan, S.L. Campbell and L.R. Petzold, Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations. North-Holland, New York (1989).
- [6] P.I. Davies and N.J. Higham, Computing f(A)b for matrix functions f. In: A. Borici, A. Frommer, B. Joo, A. Kennedy and B. Pendleton (Eds.), QCD and Numerical Analysis III, Vol. 47 of Lecture Notes in Computational Science and Engineering, Springer-Verlag, Berlin (2005), 15-24.



Figure 3: Comparison of numerical solution (curves) and analytic solution (symbols) for a space fractional diffusion equation with a radiating end  $(BC)_3$  and  $\kappa = 0.5$ ,  $\alpha = 1.9$  at t = 0.1, 0.3, 0.5, 0.7, 0.9, respectively.

- [7] R. Gorenflo and F. Mainardi, Random Walk Models for Space Fractional Diffusion Processes. *Fractional Calculus & Applied Analysis* 1, No 1 (1998), 167-191.
- [8] R. Gorenflo and F. Mainardi, Approximation of Levy-Feller Diffusion by Random Walk. *Journal for Analysis and its Applications (ZAA)* 18 (1999), 231-246.
- [9] M. Ilic, F. Liu, I. Turner and V. Anh, Numerical approximation of a fractional-in-space diffusion equation, I. Fractional Calculus & Applied Analysis 8, No 3 (2005), 323-341.
- [10] F. Liu and S. K. Bhatia, Computationally efficient solution techniques for adsorption problems involving steep gradients in bidisperse particles. *Comp. Chem. Eng.* 23 (1999), 933-943.
- [11] F. Liu and S. K. Bhatia, Numerical solution of hyperbolic models of transport in bidisperse solids. *Comp. Chem. Eng.* 24 (2000), 1981-1995.
- [12] F. Liu and S. K. Bhatia, Application of Petrov-Galerkin methods to



Figure 4: Comparison of numerical solution (curves) and analytic solution (symbols) for a space fractional diffusion equation with a radiating end  $(BC)_3$  and  $\kappa = 0.5$ ,  $\alpha = 1.8$  at t = 0.1, 0.3, 0.5, 0.7, 0.9, respectively.

transient boundary value problems in chemical engineering: Adsorption with steep gradients in bidisperse solids. *Chem. Eng. Sci.* 56 (2001), 3727-3735.

- [13] F. Liu and S. K. Bhatia, Solution techniques for transport problems involving steep concentration gradients: application to noncatalytic fluid-solid reactions. *Comp. Chem. Eng.* 25 (2001), 1159-1168.
- [14] F. Liu, I. Turner and V.V. Anh, An unstructured mesh finite volume method for modelling saltwater intrusion into coastal aquifers. *Korean J. Comp. Appl. Math.* 9 (2002), 391-407.
- [15] F. Liu, V. Anh and I. Turner, Numerical solution of the space fractional Fokker-Planck equation. J. Comp. Appl. Math. 166 (2004), 209-219.
- [16] F. Liu, V. Anh, I. Turner and P. Zhuang, Numerical simulation for solute transport in fractal porous media. ANZIAM J. 45(E) (2004), 461-473.
- [17] F. Liu, V. Anh, I. Turner, K. Bajracharya, W. Huxley and N. Su, A finite volume simulation model for saturated-unsaturated flow and ap-

plication to Gooburrum, Bundaberg, Queensland, Australia. *Applied Mathematical Modelling* **29** (2005), 852-870.

- [18] M.M. Meerschaert and C. Tadjeran, Finite difference approximations for fractional advection-dispersion flow equations. *Journal of Computational and Applied Mathematics* **172** (2004), 65-77.
- [19] R. Metzler and J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Phys. Rep.* **339** (2000), 1-77.
- [20] I. Podlubny, Fractional Differential Equations. Academic Press, N. York (1999).
- [21] S. Shen and F. Liu, Error analysis of an explicit finite difference approximation for the space fractional diffusion with insulated ends. ANZIAM J. 46(E) (2005), 871-887.
- [22] S.G. Samko, A.A. Kilbas and O.I. Marichev, Fractional Integrals and Derivatives: Theory and Applications. Gordon and Breach Science Publishers (1993).
- [23] B. West and V. Seshadri, Linear Systems With Levy Fluctuations. *Physica A* 113 (1982), 203-216.

<sup>1</sup> 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

<sup>2</sup> School of Mathematical Sciences Xiamen University, Xiamen 361005, CHINA e-mail: fwliu@xmu.edu.cn Received: June 1, 2006