Numerical methods for the fractional partial differential equations with the Riesz space fractional derivatives ⋆

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Abstract

In this paper, we consider the numerical solutions of a fractional partial differential equation with Riesz space fractional derivatives (FPDE-RSFD) on a finite domain. Two kinds of FPDE-RSFD are considered: the Riesz fractional diffusion equation (RFDE) and the Riesz fractional advection-dispersion equation (RFADE). RFDE is obtained from the standard diffusion equation by replacing the second-order space derivative with the Riesz fractional derivative of order $\alpha \in (1, 2]$; RFADE is obtained from the standard advection-dispersion equation by replacing the the first-order and second-order space derivatives with the Riesz fractional derivatives of order $\beta \in (0, 1)$ and of order $\alpha \in (1, 2]$, respectively. Firstly, analytic solutions of both RFDE and RFADE are derived. Secondly, three numerical methods are provided to deal with the Riesz space fractional derivatives, the L1/L2-approximation method, the standard/shifted Grünwald method, and a new matrix transform method (MTM). Thirdly, the RFDE and RFADE are transformed into a system of ordinary differential equations (ODE), which is then solved by the method of lines (MOL). Finally, numerical results are given, which are in good agreement with the analytic solutions.

Key words: fractional advection-dispersion equation, Riesz space fractional derivative, L1/L2-approximation method, standard/shifted Grünwald method, matrix transform method, method of lines
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1 INTRODUCTION

The concept of fractional derivatives is by no means new. In fact, they are almost as old as their more familiar integer-order counterparts [30,32,33,36]. Until recently, however, fractional derivatives have been successfully applied to problems in system biology [42], physics [1,28,29,35,43], chemistry and biochemistry [41], hydrology [2,3,15,16], and finance [9,34,37,40]. These new fractional-order models are more adequate than the previously used integer-order models, because fractional order derivatives and integrals enables the description of the memory and hereditary properties of different substances [33]. This is the most significant advantage of the fractional order models in comparison with integer order models, in which such effects are neglected. In the area of physics, fractional space derivatives are used to model anomalous diffusion or dispersion, where a particle spreads at a rate inconsistent with the classical Brownian motion model [29]. Especially, the Riesz fractional derivative includes a left Riemann-Liouville derivative and a right Riemann-Liouville derivative that allow the modelling of flow regime impacts from either side of the domain [43]. Fractional advection-dispersion equation (FADE) is used in groundwater hydrology to model the transport of passive tracers carried by fluid flow in a porous medium [15]. Benson et al. [2,3] also studied the FADE for solute transport in subsurface material. However, the analytical solutions of the fractional order partial differential equations are usually derived in terms of Green funciton or Fox funtion [10,24], and hence are difficult to evaluate. Therefore, numerical treatments and analysis of the fractional order differential equations become a fruitful research topic and have an extensive field and great potentiality.

A number of authors have discussed the numerical methods for solving the FADE with nonsymmetric fractional derivatives. Liu et al. [16] considered the time FADE and the solution was obtained using a variable transformation, together with Mellin and Laplace transforms, and H-functions. Huang and Liu [11] also considered the space-time FADE and the solution was obtained in terms of Green functions and representations of the Green function by applying the Fourier-Laplace transforms. Meerschaert and Tadjeran [26] presented practical numerical methods to solve the one-dimensional space FADE with variable coefficients on a finite domain. Liu et al. [15] transformed the space fractional Fokker-Planck equation into a system of ordinary differential equations (Method of Lines), which was then solved using backward differen-

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tiation formulas. Momani and Odibat [31] developed a reliable algorithm of the Adomian decomposition method to construct a numerical solution of the space-time FADE in the form of a rapidly convergent series with easily computable components. However, they did not give its theoretical analysis. Liu et al. [23] proposed an approximation of the Lévy-Feller advection-dispersion process by employing a random walk and finite difference methods.

The FADE with a symmetric fractional derivative, namely the Riesz fractional derivative, is derived from the kinetics of chaotic dynamics by Saichev and Zaslavsky in [35] and summerised by Zaslavsky in [43]. Ciesielski and Leszczynski [6] present a numerical solution for the Riesz FADE (without the advection term) based on the finite differences method. Meerschaert and Tadjeran [27] propose a shifted Grünwald estimate for the two-sided space fractional partial differential equations. In the light of their paper, Shen et al. [38] present explicit and implicit difference approximations for the Riesz FADE with initial and boundary conditions on a finite domain, and derive the stability and convergence of the proposed numerical methods. To the authors' best knowledge, there is no other research on the numerial methods for solving Riesz FADE. Therefore, the numerical treatments for the Riesz FADE are still spare. This motivate us to investigate more computationally efficient numerical techniques for solving Riesz FADE.

In this paper, we consider the following fractional partial differential equations with the Riesz space fractional derivatives (FPDE-RSFD):

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) + K_\beta \frac{\partial^\beta}{\partial |x|^\beta} u(x,t), \quad 0 < t \le T, \quad 0 < x < L \tag{1}$$

subject to the boundary and initial conditions given by

$$u(0,t) = u(L,t) = 0, \tag{2}$$

$$u(x,0) = g(x), \tag{3}$$

where u is, for example, a solute concentration; K_α and K_β represent the dispersion coefficient and the average fluid velocity. The Riesz space fractional derivatives of order $\alpha(1 < \alpha \le 2)$ and $\beta(0 < \beta < 1)$ are defined respectively as

$$\frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) = -c_\alpha ({}_0D_x^\alpha +_x D_L^\alpha) u(x,t), \tag{4}$$

$$\frac{\partial^\beta}{\partial |x|^\beta} u(x,t) = -c_\beta ({}_0D_x^\beta +_x D_L^\beta) u(x,t), \tag{5}$$

where

$$
\begin{aligned}
c_\alpha &= \frac{1}{2\cos(\frac{\pi\alpha}{2})}, \qquad \alpha \neq 1, \qquad c_\beta = \frac{1}{2\cos(\frac{\pi\beta}{2})}, \qquad \beta \neq 1, \\
{}_0D_x^\alpha u(x,t) &= \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_0^x \frac{u(\xi,t)d\xi}{(x-\xi)^{\alpha-1}}, \\
{}_xD_L^\alpha u(x,t) &= \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_x^L \frac{u(\xi,t)d\xi}{(\xi-x)^{\alpha-1}}, \\
{}_0D_x^\beta u(x,t) &= \frac{1}{\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_0^x \frac{u(\xi,t)d\xi}{(x-\xi)^{\beta}}, \\
{}_xD_L^\beta u(x,t) &= -\frac{1}{\Gamma(1-\beta)} \frac{\partial}{\partial x} \int_x^L \frac{u(\xi,t)d\xi}{(\xi-x)^{\beta}}.
\end{aligned}
$$

Here ${}_0D_x^\alpha$ (${}_0D_x^\beta$) and ${}_xD_L^\alpha$ (${}_xD_L^\beta$) are defined as the left- and right-side Riemann-Liouville derivatives.

The fractional kinetic equation (1) has a physical meaning (see [35,43] for further details). Physical considerations of a fractional advection-dispersion transport model restrict $1 < \alpha \leq 2$, $0 < \beta < 1$, and we assume $K_\alpha > 0$ and $K_\beta \geq 0$ so that the flow is from left to right. The physical meaning of using homogeneous Dirichlet boundary conditions is that the boundary is set far enough away from an evolving plume such that no significant concentrations reach that boundary [25,27]. In the case of $\alpha = 2$ and $\beta = 1$, Eq. (1) reduces to the classical advection-dispersion equation (ADE). In this paper, we only consider the fractional cases: when $K_\beta = 0$, Eq. (1) reduces to the Riesz fractional diffusion equation (RFDE) [35]; when $K_\beta \neq 0$, the Riesz fractional advection-dispersion equation (RFADE) is obtained [43].

There are different techniques for approximating different fractional derivatives [33,36,32]. People may get confused on this issue. One contribution of this paper is that we illustrate how to choose different techniques for different fractional derivatives. For simulation of Riemann-Liouville fractional derivative, there exists a link between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives. This allows the use of the Riemann-Liouville definition during problem formulation, and then the use of the Grünwald-Letnikov definition for obtaining the numerical solution [33]. When using the standard Grünwald approximation for the Riemann-Liouville fractional derivative, Meerschaert and Tadjeran [26] found that the standard Grünwald approximation to discretize the fractional diffusion equation results in an unstable finite difference scheme regardless of whether the resulting finite difference method is an explicit or an implicit system. In order to show how to use the standard Grünwald approximation and Shifted Grünwald approximation, we consider the the Riesz fractional advection-dispersion equation 1. We approximate the diffusion term by the shifted Grünwald method and approximate the advection term by the standard Grünwald method. In our opinion, this is a new and novel approach.

Another contribution of this paper is that we clarify the two existing definitions of the operator $\frac{\partial^\alpha}{\partial|x|^\alpha}$. One is defined on the Fourier transform on infinite domain [36], and the other one is defined through eigenfuntion expansion on a finite domain [12]. On infinite domain, we derived the equivalence of the operators $\frac{\partial^\alpha}{\partial|x|^\alpha}$ and $-(-\Delta)^{\frac{\alpha}{2}}$. We notice that this equivalence also holds on finite domain when the function $u(x)$ is subject to homogeneous Dirichlet boundary conditions. Here, we propose two numerical methods to approximate the Riesz fractional derivative: the standard/shifted Grünwald method and the L1/L2 approximation. For $\frac{\partial^\alpha}{\partial|x|^\alpha}$ defined through eigenfuntion expansion, we derive the analytic solutions of the RFDE and RFADE 1 using a spectral representation, and develop the matrix transform method (MTM) to slove the RFDE and RFADE 1. Though the definitions of fractional Laplacian are different on infinite domain and finite domain, the numerical results shows that the MTM is still an efficient approximation of the Riesz fractional derivative.

After introducing three numerical methods to estimate the Riesz fractinal derivative, we use the fractional method of lines proposed by Liu et al. [15] to transform the RFDE and RFADE into a system of time ordinary differential equations (TODEs). Then, the TODEs system is solved using a differential/algebraic system solver (DASSL) [5].

The rest of this paper is organized as follows. Section 2 presents some important definitions and lemmas used in this paper. Analytic and numerical solutions for the RFDE and RFADE are derived in Sections 3 and 4, respectively. Section 5 provides the numerical results for solving the RFDE and RFADE. Finally, the main results are summarised in Section 6.

2 PRELIMINARY KNOWLEDGE

In this section, we outline important definitions and lemma used throughout the remaining sections of this paper.

Definition 1. [8] The Riesz fractional operator for $n-1<\alpha\le n$ on a finite interval $0\le x\le L$ is defined as

$$ {}^R D_x^\alpha u(x,t) = \frac{\partial^\alpha}{\partial|x|^\alpha} u(x,t) = -c_\alpha({}_0D_x^\alpha + {}_x D_L^\alpha)u(x,t) $$

where

$$ c_\alpha = \frac{1}{2\cos(\frac{\pi\alpha}{2})}, \qquad \alpha \neq 1, $$

$$
\begin{aligned}
{}_0D_x^{\alpha}u(x,t) &= \frac{1}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_0^x \frac{u(\xi,t)d_\xi}{(x-\xi)^{\alpha+1-n}},\\
{}_xD_L^{\alpha}u(x,t) &= \frac{(-1)^n}{\Gamma(n-\alpha)}\frac{\partial^n}{\partial x^n}\int_x^L \frac{u(\xi,t)d_\xi}{(\xi-x)^{\alpha+1-n}}.
\end{aligned}
$$

Lemma 1. For a function $u(x)$ defined on the infinite domain $[-\infty < x < \infty]$, the following equality holds

$$
-(-\Delta)^{\frac{\alpha}{2}}u(x) = -\frac{1}{2\cos\frac{\pi\alpha}{2}}[{}_{-\infty}D_x^{\alpha}u(x) +_x D_{\infty}^{\alpha}u(x)] = \frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x).
$$

Proof. According to Samko et al. [36], a fractional power of the Laplace operator is defined as follows:

$$
-(-\Delta)^{\frac{\alpha}{2}}u(x) = -\mathcal{F}^{-1}|x|^{\alpha}\mathcal{F}u(x). \tag{6}
$$

where $\mathcal{F}$ and $\mathcal{F}^{-1}$ denote the Fourier transform and inverse Fourier transform of $u(x)$, respectively. Hence, we have

$$
-(-\Delta)^{\frac{\alpha}{2}}u(x) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ix\xi}|\xi|^{\alpha}\int_{-\infty}^{\infty} e^{i\xi\eta}u(\eta)d\eta d\xi.
$$

Supposing that $u(x)$ vanishes at $x = \pm\infty$, we perform integration by parts,

$$
\int_{-\infty}^{\infty} e^{i\xi\eta}u(\eta)d\eta = -\frac{1}{i\xi}\int_{-\infty}^{\infty} e^{i\xi\eta}u'(\eta)d\eta.
$$

Thus, we obtain

$$
-(-\Delta)^{\frac{\alpha}{2}}u(x) = -\frac{1}{2\pi}\int_{-\infty}^{\infty} u'(\eta)\left[i\int_{-\infty}^{\infty} e^{i\xi(\eta-x)}\frac{|\xi|^{\alpha}}{\xi}d\xi\right]d\eta.
$$

Let $I = i\int_{-\infty}^{\infty} e^{i\xi(\eta-x)}\frac{|\xi|^{\alpha}}{\xi}d\xi$, then

$$
I = i\left[-\int_0^{\infty} e^{i\xi(x-\eta)}\xi^{\alpha-1}d\xi + \int_0^{\infty} e^{i\xi(\eta-x)}\xi^{\alpha-1}d\xi\right].
$$

Noting that

$$
\mathcal{L}(t^{v-1}) = \int_0^{\infty} e^{-st}t^{v-1}d_t = \frac{\Gamma(v)}{s^v}, \qquad Re(v) > 0,
$$

for $0 < \alpha < 1$, we have

$$
I = i\left[\frac{-\Gamma(\alpha)}{[i(\eta-x)]^{\alpha}} + \frac{\Gamma(\alpha)}{[i(x-\eta)]^{\alpha}}\right] = \frac{sign(x-\eta)\Gamma(\alpha)\Gamma(1-\alpha)}{|x-\eta|^{\alpha}\Gamma(1-\alpha)}[i^{\alpha-1} + (-i)^{\alpha-1}].
$$

Using $\Gamma(\alpha)\Gamma(1-\alpha)=\frac{\pi}{\sin\pi\alpha}$ and $i^{\alpha-1}+(-i)^{\alpha-1}=2\sin\frac{\pi\alpha}{2}$, we obtain

$$I=\frac{sign(x-\eta)\pi}{\cos\frac{\pi\alpha}{2}|x-\eta|^{\alpha}\Gamma(1-\alpha)}.$$

Hence, for $0<\alpha<1$,

$$\begin{aligned}-(-\Delta)^{\frac{\alpha}{2}}u(x)&=-\frac{1}{2\pi}\int_{-\infty}^{\infty}u'(\eta)\frac{sign(x-\eta)\pi}{\cos\frac{\pi\alpha}{2}|x-\eta|^{\alpha}\Gamma(1-\alpha)}d\eta\\&=-\frac{1}{2\cos\frac{\pi\alpha}{2}}\left[\frac{1}{\Gamma(1-\alpha)}\int_{-\infty}^{x}\frac{u'(\eta)}{(x-\eta)^{\alpha}}d\eta-\frac{1}{\Gamma(1-\alpha)}\int_{x}^{\infty}\frac{u'(\eta)}{(\eta-x)^{\alpha}}d\eta\right].\end{aligned}$$

Following [33], for $0<\alpha<1$, the Grünwald-Letnikov fractional derivative in $[a,x]$ is given by

$${}_aD_x^{\alpha}u(x)=\frac{u(a)(x-a)^{-\alpha}}{\Gamma(1-\alpha)}+\frac{1}{\Gamma(1-\alpha)}\int_{a}^{x}\frac{u'(\eta)}{(x-\eta)^{\alpha}}d\eta.$$

Therefore, if $u(x)$ tends to be zero for $a\to-\infty$, then we have

$${}_{-\infty}D_x^{\alpha}u(x)=\frac{1}{\Gamma(1-\alpha)}\int_{-\infty}^{x}\frac{u'(\eta)}{(x-\eta)^{\alpha}}d\eta.$$

Similarly, if $u(x)$ tends to be zero for $b\to\infty$, then we have

$${}_xD_{\infty}^{\alpha}u(x)=\frac{-1}{\Gamma(1-\alpha)}\int_{x}^{\infty}\frac{u'(\eta)}{(\eta-x)^{\alpha}}d\eta.$$

Hence, if $u(x)$ is continuous and $u'(x)$ is integrable for $x\geq a$, then for every α $(0<\alpha<1)$, the Riemann-Liouville derivative exists and coincides with the Grünwald-Letnikov derivative. Finally, for $0<\alpha<1$, we have

$$-(-\Delta)^{\frac{\alpha}{2}}u(x)=-\frac{1}{2\cos\frac{\pi\alpha}{2}}[{}_{-\infty}D_x^{\alpha}u(x)+{}_xD_{\infty}^{\alpha}u(x)]=\frac{\partial^{\alpha}}{\partial|x|^{\alpha}}u(x),$$

where

$$\begin{aligned}{}_{-\infty}D_x^{\alpha}u(x)&=\frac{1}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_{-\infty}^{x}\frac{u(\eta)d\eta}{(x-\eta)^{\alpha}},\\{}_xD_{\infty}^{\alpha}u(x)&=\frac{-1}{\Gamma(1-\alpha)}\frac{\partial}{\partial x}\int_{x}^{\infty}\frac{u(\eta)d\eta}{(\eta-x)^{\alpha}}.\end{aligned}$$

Next, we present here a similar derivation for the case of $1<\alpha<2$. Supposing that $u(x)$,$u'(x)$, vanishes at $x=\pm\infty$, we perform integration by parts twice, to obtain

$$\int_{-\infty}^{\infty}e^{i\xi\eta}u(\eta)d\eta=-\xi^{-2}\int_{-\infty}^{\infty}e^{i\xi\eta}u''(\eta)d\eta.$$

Hence, we have

$$
\begin{aligned}
-(-\Delta)^{\frac{\alpha}{2}}u(x) &= -\frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-ix\xi}|\xi|^{\alpha}\left[-\xi^{-2}\int_{-\infty}^{\infty} e^{i\xi\eta}u''(\eta)d\eta\right]d\xi \\
&= \frac{1}{2\pi}\int_{-\infty}^{\infty} u''(\eta)\left[\int_{-\infty}^{\infty} e^{i\xi(\eta-x)}|\xi|^{\alpha-2}d\xi\right]d\eta.
\end{aligned}
$$

Let $I=\int_{-\infty}^{\infty} e^{i\xi(\eta-x)}|\xi|^{\alpha-2}d\xi$, then

$$
I=\int_0^{\infty} e^{i\xi(x-\eta)}\xi^{\alpha-2}d\xi+\int_0^{\infty} e^{i\xi(\eta-x)}\xi^{\alpha-2}d\xi.
$$

Noting that

$$
\mathcal{L}(t^{v-2})=\int_0^{\infty} e^{-st}t^{v-2}d_t=\frac{\Gamma(v-1)}{s^{v-1}}, \qquad Re(v)>1,
$$

we have

$$
I=\frac{\Gamma(\alpha-1)}{[i(\eta-x)]^{\alpha-1}}+\frac{\Gamma(\alpha-1)}{[i(x-\eta)]^{\alpha-1}}=\frac{\Gamma(\alpha-1)\Gamma(2-\alpha)}{|x-\eta|^{\alpha-1}\Gamma(2-\alpha)}[i^{\alpha-1}+(-i)^{\alpha-1}].
$$

Using $\Gamma(\alpha-1)\Gamma(2-\alpha)=\frac{\pi}{\sin\pi(\alpha-1)}=\frac{-\pi}{\sin\pi\alpha}$ and $i^{\alpha-1}+(-i)^{\alpha-1}=2\sin\frac{\pi\alpha}{2}$, we have

$$
I=\frac{-\pi}{\cos\frac{\pi\alpha}{2}|x-\eta|^{\alpha-1}\Gamma(2-\alpha)}.
$$

Hence, for $1<\alpha<2$,

$$
\begin{aligned}
-(-\Delta)^{\frac{\alpha}{2}}u(x) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} u''(\eta)\frac{-\pi}{\cos\frac{\pi\alpha}{2}|x-\eta|^{\alpha-1}\Gamma(2-\alpha)}d\eta \\
&= -\frac{1}{2\cos\frac{\pi\alpha}{2}}\left[\frac{1}{\Gamma(2-\alpha)}\int_{-\infty}^{x}\frac{u''(\eta)}{(x-\eta)^{\alpha-1}}d\eta+\frac{1}{\Gamma(2-\alpha)}\int_{x}^{\infty}\frac{u''(\eta)}{(\eta-x)^{\alpha-1}}d\eta\right].
\end{aligned}
$$

Following [33], for $1<\alpha<2$, the Grünwald-Letnikov fractional derivative in $[a,x]$ is given by

$$
{}_aD_x^{\alpha}u(x)=\frac{u(a)(x-a)^{-\alpha}}{\Gamma(1-\alpha)}+\frac{u'(a)(x-a)^{1-\alpha}}{\Gamma(2-\alpha)}+\frac{1}{\Gamma(2-\alpha)}\int_a^x\frac{u''(\eta)}{(x-\eta)^{\alpha-1}}d\eta.
$$

Therefore, if $u(x)$ and $u'(x)$ tend to be zero for $a\rightarrow-\infty$, then we have

$$
{}_{-\infty}D_x^{\alpha}u(x)=\frac{1}{\Gamma(2-\alpha)}\int_a^x\frac{u''(\eta)}{(x-\eta)^{\alpha-1}}d\eta.
$$

Similarly, if $u(x)$ and $u'(x)$ tend to be zero for $b\rightarrow\infty$, then we have

$$
{}_xD_{\infty}^{\alpha}u(x)=\frac{1}{\Gamma(2-\alpha)}\int_x^{\infty}\frac{u''(\eta)}{(\eta-x)^{\alpha-1}}d\eta.
$$

Hence, if $u(x)$ and $u'(x)$ are continuous and $u''(x)$ is integrable for $x \geq a$, then for every α $(1 < \alpha < 2)$, the Riemann-Liouville derivative exists and coincides with the Grünwald-Letnikov derivative. Finally, for $1 < \alpha < 2$, we have

$$-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2\cos\frac{\pi\alpha}{2}}[{}_{-\infty}D_x^\alpha u(x) +_x D_\infty^\alpha u(x)] = \frac{\partial^\alpha}{\partial |x|^\alpha} u(x),$$

where

$${}_{-\infty}D_x^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^x \frac{u(\eta)d\eta}{(x-\eta)^{\alpha-1}},$$

$${}_x D_\infty^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_x^\infty \frac{u(\eta)d\eta}{(\eta-x)^{\alpha-1}}.$$

Further, if $n-1 < \alpha < n$, then

$$-(-\Delta)^{\frac{\alpha}{2}} u(x) = -\frac{1}{2\cos\frac{\pi\alpha}{2}}[{}_{-\infty}D_x^\alpha u(x) +_x D_\infty^\alpha u(x)] = \frac{\partial^\alpha}{\partial |x|^\alpha} u(x),$$

where

$${}_{-\infty}D_x^\alpha u(x) = \frac{1}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_{-\infty}^x \frac{u(\eta)d\eta}{(x-\eta)^{\alpha+1-n}},$$

$${}_x D_\infty^\alpha u(x) = \frac{(-1)^n}{\Gamma(n-\alpha)} \frac{\partial^n}{\partial x^n} \int_x^\infty \frac{u(\eta)d\eta}{(\eta-x)^{\alpha+1-n}}.$$

Remark 1. For a function $u(x)$ given in a finite interval $[0, L]$, the above equality also holds when setting

$$u^*(x) = \begin{cases} u(x) & x \in (0, L), \\ 0 & x \notin (0, L), \end{cases}$$

i.e., $u^*(x) = 0$ on the boundary points and beyond the boundary points.

Definition 2. [13] Suppose the Laplacian $(-\Delta)$ has a complete set of orthonormal eigenfunctions φ_n corresponding to eigenvalues λ_n^2 on a bounded region $\mathcal{D}$, i.e., $(-\Delta)\varphi_n = \lambda_n^2 \varphi_n$ on a bounded region $\mathcal{D}$; $\mathcal{B}(u) = 0$ on $\partial\mathcal{D}$, where $\mathcal{B}(u)$ represents homogeneous Dirichlet 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

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

3 ANALYTIC SOLUTION AND NUMERICAL METHODS OF THE RFDE

In this section, we consider the following Riesz fractional diffusion equation (RFDE):

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t), \quad 0 < t \leq T, \quad 0 < x < L, \quad 1 < \alpha \leq 2 \tag{7}$$

with the boundary and initial conditions given by

$$u(0,t) = u(L,t) = 0, \tag{8}$$
$$u(x,0) = g(x). \tag{9}$$

Firstly, we derive the analytic solution of the RFDE in Section 3.1, and then introduce three different numerical methods for solving the RFDE in Sections 3.2-3.4.

3.1 Analytic solution for the RFDE

In this subsection, we present a spectral representation for the RFDE. Following Lemma 1, we first recognize that

$$\frac{\partial^\alpha u}{\partial |x|^\alpha} = -(-\Delta)^{\frac{\alpha}{2}} u,$$

for the function $u(x)$ on a finite domain $[0, L]$ with homogeneous Dirichlet boundary values. Hence, the RFDE (7) can be expressed in the form

$$\frac{\partial u(x,t)}{\partial t} = -K_\alpha (-\Delta)^{\frac{\alpha}{2}} u(x,t). \tag{10}$$

The spectral representation of the Laplacian operator $(-\Delta)$ is obtained by solving the eigenvalue problem:

$$-\Delta\varphi = \lambda\varphi,$$
$$\varphi(0) = \varphi(L) = 0.$$

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 $\varphi_n(x) = \sin(\frac{n\pi x}{L})$. Next, the solution is given by

$$u(x,t) = \sum_{n=1}^{\infty} c_n(t) \sin(\frac{n\pi x}{L}),$$

which automatically satisfies the boundary condition (8). Using Definition 2 and substituting $u(x,t)$ into Eq.(10), we obtain

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

The problem for c_n becomes into a system of ordinary differential equations

$$\frac{dc_n}{dt} + K_\alpha(\lambda_n)^{\frac{\alpha}{2}} c_n = 0,$$

which has the general solution

$$c_n(t) = c_n(0) \exp(-K_\alpha(\lambda_n)^{\frac{\alpha}{2}} t).$$

To obtain $c_n(0)$ we use the initial condition (9)

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

from which we deduce that

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

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

$$u(x,t) = \sum_{n=1}^{\infty} b_n \sin(\frac{n\pi x}{L}) \exp(-K_\alpha(\frac{n^2\pi^2}{L^2})^{\frac{\alpha}{2}} t). \quad (11)$$

3.2 L2-approximation method for the RFDE

In this section, we provide a numerical solution of the RFDE by the $L2$-approximation method. In Section 1, the Riesz fractional derivative of order $1 < \alpha \leq 2$ on a finite interval $[0, L]$ was defined in the sense of the Riemann-Liouville definition. There is another very important definition for the fractional derivative, namely, the Grünwald-Letnikov definition. For $1 < \alpha \leq 2$, the left- and right-handed Grünwald-Letnikov fractional derivatives on $[0, L]$

are, respectively, given by

$$
{}_0D_x^\alpha u(x) = \frac{u(0)x^{-\alpha}}{\Gamma(1-\alpha)} + \frac{u'(0)x^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\int_0^x \frac{u^{(2)}(\xi)d\xi}{(x-\xi)^{\alpha-1}}, \tag{12}
$$

$$
{}_xD_L^\alpha u(x) = \frac{u(L)(L-x)^{-\alpha}}{\Gamma(1-\alpha)} + \frac{u'(L)(L-x)^{1-\alpha}}{\Gamma(2-\alpha)} + \frac{1}{\Gamma(2-\alpha)}\int_x^L \frac{u^{(2)}(\xi)d\xi}{(\xi-x)^{\alpha-1}}. \tag{13}
$$

Following [33], there exists a link between these two approaches to differentiation of arbitrary real order. Let us suppose that the function $u(x)$ is $n-1$ times continuously differentiable in the interval $[0, L]$ and that $u^{(n)}(x)$ is integrable in $[0, L]$. Then for every α $(0 \le n-1 < \alpha < n)$ the Riemann-Liouville derivative exists and coincides with the Grünwald-Letnikov derivative. This relationship between the Riemann-Liouville and Grünwald-Letnikov definitions allows the use of the Riemann-Liouville definition during the problem formulation, and then the Grünwald-Letnikov definition for obtaining the numerical solution [15]. Therefore, using the link between these two definitions and the $L2$-algorithm proposed by [15,32], we can easily obtain the following numerical discretization scheme for the RFDE.

Assume that the spatial domain is $[0, L]$. The mesh is N equal intervals of $h = L/N$ and $x_l = lh$ for $0 \le l \le N$.

The second term of the right-hand side of Eq. (12) can be approximated by

$$
\frac{u'(0)x^{1-\alpha}}{\Gamma(2-\alpha)} \approx \frac{h^{-\alpha}}{\Gamma(2-\alpha)l^{\alpha-1}}(u_1 - u_0).
$$

The third term of the right-hand side of Eq. (12) can be approximated by

$$
\begin{aligned}
&\frac{1}{\Gamma(2-\alpha)}\int_0^x \frac{u^{(2)}(\xi)d\xi}{(x-\xi)^{\alpha-1}} = \frac{1}{\Gamma(2-\alpha)}\int_0^x \frac{u^{(2)}(x-\xi)d\xi}{\xi^{\alpha-1}} \\
=&\frac{1}{\Gamma(2-\alpha)}\sum_{j=0}^{l-1}\int_{jh}^{(j+1)h}\frac{u^{(2)}(x-\xi)d\xi}{\xi^{\alpha-1}} \\
\approx&\frac{1}{\Gamma(2-\alpha)}\sum_{j=0}^{l-1}\frac{u(x-(j-1)h) - 2u(x-jh) + u(x-(j+1)h)}{h^2}\int_{jh}^{(j+1)h}\frac{d\xi}{\xi^{\alpha-1}} \\
=&\frac{h^{-\alpha}}{\Gamma(3-\alpha)}\sum_{j=0}^{l-1}(u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}].
\end{aligned}
$$

Hence, we obtain an approximation of the left-handed fractional derivative

(12) with $1 < \alpha \leq 2$ as

$$
\begin{aligned}
{}_0D_x^{\alpha}u(x_l) \approx \frac{h^{-\alpha}}{\Gamma(3-\alpha)}\Bigg\{ & \frac{(1-\alpha)(2-\alpha)u_0}{l^{\alpha}} + \frac{(2-\alpha)(u_1-u_0)}{l^{\alpha-1}} \\
& + \sum_{j=0}^{l-1}(u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}]\Bigg\}. \qquad (14)
\end{aligned}
$$

Similarly, we can derive an approximation of the right-handed fractional derivative (13) with $1 < \alpha \leq 2$ as

$$
\begin{aligned}
{}_xD_L^{\alpha}u(x_l) \approx \frac{h^{-\alpha}}{\Gamma(3-\alpha)}\Bigg\{ & \frac{(1-\alpha)(2-\alpha)u_N}{(N-l)^{\alpha}} + \frac{(2-\alpha)(u_N-u_{N-1})}{(N-l)^{\alpha-1}} \\
& + \sum_{j=0}^{N-l-1}(u_{l+j-1} - 2u_{l+j} + u_{l+j+1})[(j+1)^{2-\alpha} - j^{2-\alpha}]\Bigg\}. \qquad (15)
\end{aligned}
$$

Therefore, using the fractional Grünwald-Letnikov definitions (12) and (13), together with the numerical approximations (14) and (15), the RFDE (7) can be cast into the following system of time ordinary differential equations (TODEs):

$$
\begin{aligned}
\frac{du_l}{dt} \approx -\frac{K_{\alpha}h^{-\alpha}}{2\cos(\frac{\pi\alpha}{2})\Gamma(3-\alpha)}\Bigg\{ & \frac{(1-\alpha)(2-\alpha)u_0}{l^{\alpha}} + \frac{(2-\alpha)}{l^{\alpha-1}}(u_1-u_0) \\
& + \sum_{j=0}^{l-1}(u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}] \\
& + \frac{(1-\alpha)(2-\alpha)u_N}{(N-l)^{\alpha}} + \frac{(2-\alpha)}{(N-l)^{(\alpha-1)}}(u_N - u_{N-1}) \\
& + \sum_{j=0}^{N-l-1}(u_{l+j-1} - 2u_{l+j} + u_{l+j+1})[(j+1)^{2-\alpha} - j^{2-\alpha}]\Bigg\}. \qquad (16)
\end{aligned}
$$

A number of efficient techniques for implementing Eq.(16) have been previously proposed [5,7,14,39]. Brenan et al. [5] 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 TODEs solver. This technique has been used by many researchers when solving adsorption problems involving step gradients in bidisperse solids [4,17,19], hyperbolic models of transport in bidisperse solids [18], transport problems involving steep concentration gradients [20], and modelling saltwater intrusion into coastal aquifers [21,22].

3.3 Shifted Grünwald approximation method for the RFDE

The shifted Grünwald formula for discretizing the two-sided fractional derivative is proposed by Meerschaert and Tadjeran [27], and it was shown that the standard (i.e., unshifted) Grünwald formula to discretize the fractional diffusion equation results in an unstable finite difference scheme regardless of whether the resulting finite difference method is an explicit or an implicit system. Hence, in this section, we discretise the Riesz fractional derivative $\frac{\partial^\alpha}{\partial|x|^\alpha}u$ by the shifted Grünwald formulae [27]:

$$
{}_0D_x^\alpha u(x_l) = \frac{1}{h^\alpha}\sum_{j=0}^{l+1} g_j u_{l-j+1} + O(h), \tag{17}
$$

$$
{}_xD_L^\alpha u(x_l) = \frac{1}{h^\alpha}\sum_{j=0}^{N-l+1} g_j u_{l+j-1} + O(h), \tag{18}
$$

where the coefficients are defined by

$$
g_0 = 1, \qquad g_j = (-1)^j \frac{\alpha(\alpha-1)...(\alpha-j+1)}{j!}
$$

for $j = 1, 2, ..., N$. Then the RFDE (7) can be cast into the following system of time ordinary differential equations (TODEs):

$$
\frac{du_l}{dt} \approx -\frac{K_\alpha}{2\cos(\frac{\pi\alpha}{2})h^\alpha}\left[\sum_{j=0}^{l+1} g_j u_{l-j+1} + \sum_{j=0}^{N-l+1} g_j u_{l+j-1}\right], \tag{19}
$$

which can also be solved by DASSL.

3.4 Matrix transform method for the RFDE

Ilić et al. [12] proposed the Matrix transform method (MTM) for a space fractional diffusion equation with homogeneous boundary conditions. They have shown that the MTM provides the best approximation to the analytical solution. In this section, we apply this new technique to the RFDE. Following [12], we approximate Eq.(10) by the matrix representation:

$$
\frac{\partial \mathbf{U}}{\partial t} = -\eta \mathbf{A}^{\frac{\alpha}{2}}\mathbf{U}, \tag{20}
$$

where $\eta = \frac{K_\alpha}{h^\alpha}$, h is the discrete spatial step defined as $h = \frac{L}{N}$, and $\mathbf{U} \in \mathbb{R}^{N-1}$, $\mathbf{A} \in \mathbb{R}^{N-1 \times N-1}$ are given respectively by

$$\mathbf{U} = \begin{bmatrix} u_1 \\ \vdots \\ u_{N-1} \end{bmatrix}, \mathbf{A} = \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}.$$

The matrix $\mathbf{A}$ is symmetric positive definite (SPD), and therefore there exits a nonsingular matrix $\mathbf{P} \in \mathbb{R}^{N-1 \times N-1}$ such that

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

where $\mathbf{\Lambda} = diag(\lambda_1, \lambda_2, \cdots, \lambda_{N-1}),\ \lambda_i(i = 1, 2, \cdots, N-1)$ being the eigenvalues of $\mathbf{A}$.

Hence, Eq.(20) becomes the following system of TODEs:

$$\frac{\partial \mathbf{U}}{\partial t} = -\eta(\mathbf{P}\mathbf{\Lambda}^{\frac{\alpha}{2}}\mathbf{P}^{\mathbf{T}})\mathbf{U}, \tag{21}$$

and initially, we have

$$\mathbf{U}(0) = [g(h), g(2h), \ldots, g((N-1)h)]^T. \tag{22}$$

DASSL can again be used as the solver for this TODEs system.

4 ANALYTIC SOLUTION AND NUMERICAL METHODS FOR THE RFADE

In this section, we consider the following Riesz fractional advection-dispersion equation (RFADE):

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) + K_\beta \frac{\partial^\beta}{\partial |x|^\beta} u(x,t),\ 0 < t \le T,\ 0 < x < L \tag{23}$$

with the boundary and initial conditions given by

$$u(0,t) = u(L,t) = 0, \tag{24}$$

$$u(x,0) = g(x), \tag{25}$$

where $K_\alpha \neq 0$, $K_\beta \neq 0$, $1 < \alpha \leq 2$, $0 < \beta < 1$. Firstly, the analytic solution is provided in Section 4.1, and then we introduce three different numerical methods for solving the RFADE in Sections 4.2-4.4.

4.1 Analytic solution for the RFADE

In this subsection, we present a spectral representation for the RFADE (23). Following Lemma 1, we first recognize that

$$\frac{\partial^\alpha u}{\partial |x|^\alpha} = -(-\Delta)^{\frac{\alpha}{2}} u \quad \text{and} \quad \frac{\partial^\beta u}{\partial |x|^\beta} = -(-\Delta)^{\frac{\beta}{2}} u$$

for the function $u(x)$ on a finite domain $[0, L]$ with homogeneous Dirichlet boundary values. Hence, the RFADE (23) can be expressed in the form

$$\frac{\partial u(x,t)}{\partial t} = -K_\alpha(-\Delta)^{\frac{\alpha}{2}} u(x,t) - K_\beta(-\Delta)^{\frac{\beta}{2}} u(x,t). \tag{26}$$

Next, set

$$u(x,t) = \sum_{n=1}^{\infty} c_n(t) \sin(\frac{n\pi x}{L}),$$

which automatically satisfies the boundary conditions (24). Using Definition 2 and substituting $u(x,t)$ into equation (26), we obtain

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

The problem for c_n becomes

$$\frac{dc_n}{dt} + [K_\alpha(\lambda_n)^{\frac{\alpha}{2}} + K_\beta(\lambda_n)^{\frac{\beta}{2}}]c_n = 0,$$

which has the general solution

$$c_n(t) = c_n(0)\exp(-[K_\alpha(\lambda_n)^{\frac{\alpha}{2}} + K_\beta(\lambda_n)^{\frac{\beta}{2}}]t).$$

To obtain $c_n(0)$, we use the initial condition (25)

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

which gives

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

Hence, the solution for the distribution function is given as:

$$u(x,t) = \sum_{n=1}^{\infty} b_n \sin(\frac{n\pi x}{L}) \exp(-[K_\alpha(\lambda_n)^{\frac{\alpha}{2}} + K_\beta(\lambda_n)^{\frac{\beta}{2}}]t), \tag{27}$$

where $\lambda_n = \frac{n^2\pi^2}{L^2}$.

4.2 L1- and L2-approximation method for the RFADE

In this section, we approximate the diffusion term by the L2-algorithm as presented in Section 3.2, and estimate the advection term by the L1-algorithm as follows.

For $0 < \beta < 1$, the left- and right-handed Grünwald-Letnikov fractional derivatives on $[0, L]$ are, respectively, given by

$${}_0D_x^\beta u(x) = \frac{u(0)x^{-\beta}}{\Gamma(1-\beta)} + \frac{1}{\Gamma(1-\beta)} \int_0^x \frac{u'(\xi)d\xi}{(x-\xi)^\beta}, \tag{28}$$

$${}_xD_L^\beta u(x) = \frac{u(L)(L-x)^{-\beta}}{\Gamma(1-\beta)} + \frac{1}{\Gamma(1-\beta)} \int_x^L \frac{u'(\xi)d\xi}{(\xi-x)^\beta}. \tag{29}$$

Using the link between the Riemann-Liouville and Grünwald-Letnikov fractional derivatives [33], the second term of the right-hand side of Eq.(28) can be approximated by

$$\begin{aligned}
&\frac{1}{\Gamma(1-\beta)} \int_0^x \frac{u'(\xi)d\xi}{(x-\xi)^\beta} = \frac{1}{\Gamma(1-\beta)} \int_0^x \frac{u'(x-\xi)d\xi}{\xi^\beta} \\
=&\frac{1}{\Gamma(1-\beta)} \sum_{j=0}^{l-1} \int_{jh}^{(j+1)h} \frac{u'(x-\xi)d\xi}{\xi^\beta} \\
\approx&\frac{1}{\Gamma(1-\beta)} \sum_{j=0}^{l-1} \frac{u(x-jh)-u(x-(j+1)h)}{h} \int_{jh}^{(j+1)h} \frac{d\xi}{\xi^\beta} \\
=&\frac{h^{-\beta}}{\Gamma(2-\beta)} \sum_{j=0}^{l-1} (u_{l-j} - u_{l-j-1})[(j+1)^{1-\beta} - j^{1-\beta}].
\end{aligned}$$

Hence, we obtain an approximation of the left-handed fractional derivative

(28) with $0 < \beta < 1$ as

$$ {}_0D_x^{\beta} u(x_l) \approx \frac{h^{-\beta}}{\Gamma(2-\beta)} \left\{ \frac{(1-\beta)u_0}{l^{\beta}} + \sum_{j=0}^{l-1} (u_{l-j} - u_{l-j-1})[(j+1)^{1-\beta} - j^{1-\beta}] \right\}. \tag{30} $$

Similarly, we can derive an approximation of the right-handed fractional derivative (29) with $0 < \beta < 1$ as

$$ {}_xD_L^{\beta} u(x_l) \approx \frac{h^{-\beta}}{\Gamma(2-\beta)} \left\{ \frac{(1-\beta)u_N}{(N-l)^{\beta}} + \sum_{j=0}^{N-l-1} (u_{l+j} - u_{l+j+1})[(j+1)^{1-\beta} - j^{1-\beta}] \right\}. \tag{31} $$

Using the numerical approximations (30) and (31), the advection term of the RFADE (23) can be approximated by

$$ \begin{aligned} K_{\beta} \frac{\partial^{\beta}}{\partial |x|^{\beta}} u(x_l) \approx & -\frac{K_{\beta} h^{-\beta}}{2\cos(\frac{\pi\beta}{2})\Gamma(2-\beta)} \left\{ \frac{(1-\beta)u_0}{l^{\beta}} \right. \\ & + \sum_{j=0}^{l-1} (u_{l-j-1} - u_{l-j})[(j+1)^{1-\beta} - j^{1-\beta}] + \frac{(1-\beta)u_N}{(N-l)^{\beta}} \\ & \left. + \sum_{j=0}^{N-l-1} (u_{l+j+1} - u_{l+j})[(j+1)^{1-\beta} - j^{1-\beta}] \right\}. \end{aligned} \tag{32} $$

Therefore, using the numerical approximation of the diffusion term (16) and the numerical approximation of the advection term (32), we transform the RFADE (23) into the following system of TODEs

$$ \begin{aligned} \frac{du_l}{dt} \approx & -\frac{K_{\alpha} h^{-\alpha}}{2\cos(\frac{\pi\alpha}{2})\Gamma(3-\alpha)} \left\{ \frac{(1-\alpha)(2-\alpha)u_0}{l^{\alpha}} + \frac{(2-\alpha)}{l^{\alpha-1}}(u_1 - u_0) \right. \\ & + \sum_{j=0}^{l-1} (u_{l-j+1} - 2u_{l-j} + u_{l-j-1})[(j+1)^{2-\alpha} - j^{2-\alpha}] \\ & + \frac{(1-\alpha)(2-\alpha)u_N}{(N-l)^{\alpha}} + \frac{(2-\alpha)}{(N-l)^{(\alpha-1)}}(u_N - u_{N-1}) \\ & \left. + \sum_{j=0}^{N-l-1} (u_{l+j-1} - 2u_{l+j} + u_{l+j+1})[(j+1)^{2-\alpha} - j^{2-\alpha}] \right\} \\ & - \frac{K_{\beta} h^{-\beta}}{2\cos(\frac{\pi\beta}{2})\Gamma(2-\beta)} \left\{ \frac{(1-\beta)u_0}{l^{\beta}} \right. \\ & + \sum_{j=0}^{l-1} (u_{l-j-1} - u_{l-j})[(j+1)^{1-\beta} - j^{1-\beta}] + \frac{(1-\beta)u_N}{(N-l)^{\beta}} \\ & \left. + \sum_{j=0}^{N-l-1} (u_{l+j+1} - u_{l+j})[(j+1)^{1-\beta} - j^{1-\beta}] \right\}. \end{aligned} \tag{33} $$

This system of TODEs is then solved using the standard ODE solver, DASSL.

4.3 Shifted and standard Grünwald approximation method for the RFADE

In this section, we approximate the diffusion term by the shifted Grünwald method as presented in Section 3.3, and estimate the advection term by the standard Grünwald formulae [33] as follows:

$$
{}_0D_x^{\beta}u(x_l) = \frac{1}{h^{\beta}}\sum_{j=0}^{l} w_j u_{l-j} + O(h), \quad {}_xD_L^{\beta}u(x_l) = \frac{1}{h^{\beta}}\sum_{j=0}^{N-l} w_j u_{l+j} + O(h),
$$

where the coefficients are defined by

$$
w_0 = 1, \qquad w_j = (-1)^j \frac{\beta(\beta-1)...(\beta-j+1)}{j!},
$$

for $j = 1, 2, ..., N$. If we approximate both the diffusion and advection terms by the shifted Grnwald method or by the standard Grnwald method, then unstable solutions will be obtained.

Then, the RFADE (23) can be cast into the following system of time ordinary differential equations (TODEs):

$$
\begin{aligned}
\frac{du_l}{dt} \approx & -\frac{K_\alpha}{2\cos(\frac{\pi\alpha}{2})h^\alpha}\left[\sum_{j=0}^{l+1} g_j u_{l-j+1} + \sum_{j=0}^{N-l+1} g_j u_{l+j-1}\right] \\
& -\frac{K_\beta}{2\cos(\frac{\pi\beta}{2})h^\beta}\left[\sum_{j=0}^{l} w_j u_{l-j} + \sum_{j=0}^{N-l} w_j u_{l+j}\right],
\end{aligned} \tag{34}
$$

which can again be solved using DASSL.

4.4 Matrix transform method for the RFADE

The matrix transform technique presented in Section 3.4 can be easily applied to the advection term $\frac{\partial^\beta u}{\partial |x|^\beta}$ $(0 < \beta < 1)$. Hence, we obtain the matrix representation for the RFADE (23) as follows:

$$
\frac{\partial \mathbf{U}}{\partial t} = -\eta_\alpha \mathbf{A}^{\frac{\alpha}{2}}\mathbf{U} - \gamma_\beta \mathbf{A}^{\frac{\beta}{2}}\mathbf{U} = -\eta_\alpha(\mathbf{P}\mathbf{\Lambda}^{\frac{\alpha}{2}}\mathbf{P}^{\mathbf{T}})\mathbf{U} - \gamma_\beta(\mathbf{P}\mathbf{\Lambda}^{\frac{\beta}{2}}\mathbf{P}^{\mathbf{T}})\mathbf{U},
$$

where $\eta_\alpha = \frac{K_\alpha}{h^\alpha}$, $\gamma_\beta = \frac{K_\beta}{h^\beta}$, $h = \frac{L}{N}$; $\mathbf{U} \in \mathbb{R}^{N-1}$, $\mathbf{A} \in \mathbb{R}^{N-1\times N-1}$ and $\mathbf{P} \in \mathbb{R}^{N-1\times N-1}$ are defined in Section 3.4; and $\mathbf{U}(0)$ is as given in Eq.(22). DASSL can again be used as the solver for this TODEs system.

5 NUMERICAL RESULTS OF THE RFDE AND RFADE

In this section, we provide numerical examples for the RFDE and RFADE to determine the accuracy of the numerical methods in comparison to the analytic solutions presented throughout Sections 3 and 4. We also use our solution methods to demonstrate the changes in solution behaviour that arise when the exponent is varied from integer order to fractional order, and to identify the differences between solutions with and without the advection term.

5.1 Numerical examples of the RFDE

In this subsection, we present two examples of the RFDE on a finite domain $[0, \pi]$. Firstly, we consider the following equation

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t), \quad 0 < t \le T, \quad 0 < x < \pi \tag{35}$$

with the initial and boundary conditions given by

$$u(x,0) = x^2(\pi - x), \tag{36}$$

$$u(0,t) = u(\pi,t) = 0. \tag{37}$$

According to Section 3.1,

$$\begin{aligned} b_n = c_n(0) &= \frac{2}{\pi}\int_0^\pi g(\xi)\sin(\frac{n\pi\xi}{\pi})d\xi = \frac{2}{\pi}\int_0^\pi \xi^2(\pi-\xi)\sin(n\xi)d\xi \\ &= \frac{8}{n^3}(-1)^{n+1} - \frac{4}{n^3}. \end{aligned}$$

Hence, the analytic solution of Eq.(35)-(37) is given by

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

In Figure 1, this analytic solution is compared with the three numerical methods proposed in Sections 3.2-3.4, for $t = 0.4$, $\alpha = 1.8$ and $K_\alpha = 0.25$. It can be seen that all three numerical methods perform well. However, from Table

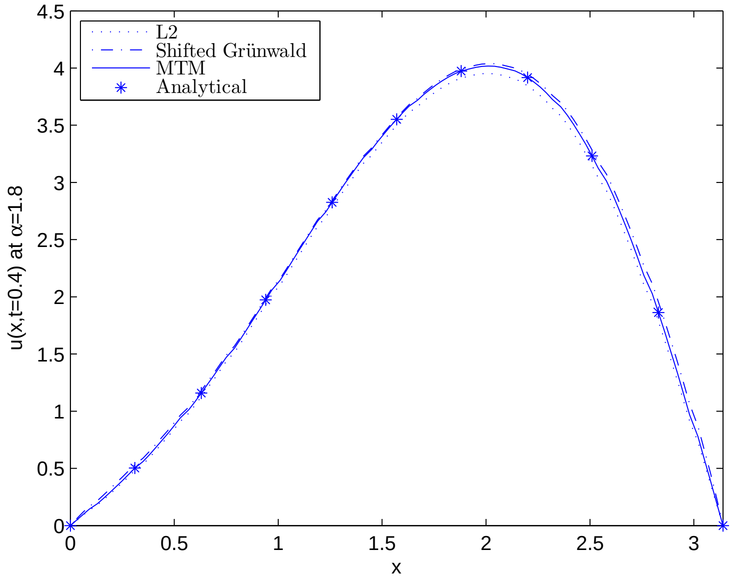

Fig. 1. Comparison of the numerical solutions with the analytic solution at $t = 0.4$ for the RFDE (35)-(37) with $K_\alpha = 0.25$ and $\alpha = 1.8$.

Table 1
Maximum errors for 3 methods when $0 < x < \pi$

$h = \pi/N$	L_2 approximation	Matrix transform	Shifted Grünwald
$\pi/10$	9.471E-2	2.217E-2	6.726E-2
$\pi/20$	9.472E-2	5.759E-3	7.343E-2
$\pi/40$	9.041E-2	1.481E-3	8.693E-2
$\pi/80$	8.604E-2	3.727E-4	9.535E-2

1, we see that, among three methods, only the matrix transform method is stable and convergent. Using the matrix method from Section 3.4, The solution profiles of RFDE for different values of $\alpha = 1.2, 1.4, 1.6, 1.8, 2.0$ when $t = 0.5, 1.5, 2.5, 3.5$ are shown in Figure 2. It can be seen that the process described by the RFDE is slightly more skewed to the right than that modelled by the standard diffusion equation.

To further demonstrate the impact of fractional order to the solution behaviour, another example of RFDE with a different initial condition is now considered:

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t), \quad 0 < t \le T, \quad 0 < x < \pi, \tag{38}$$

$$u(x,0) = \sin 4x, \tag{39}$$

$$u(0,t) = u(\pi,t) = 0. \tag{40}$$

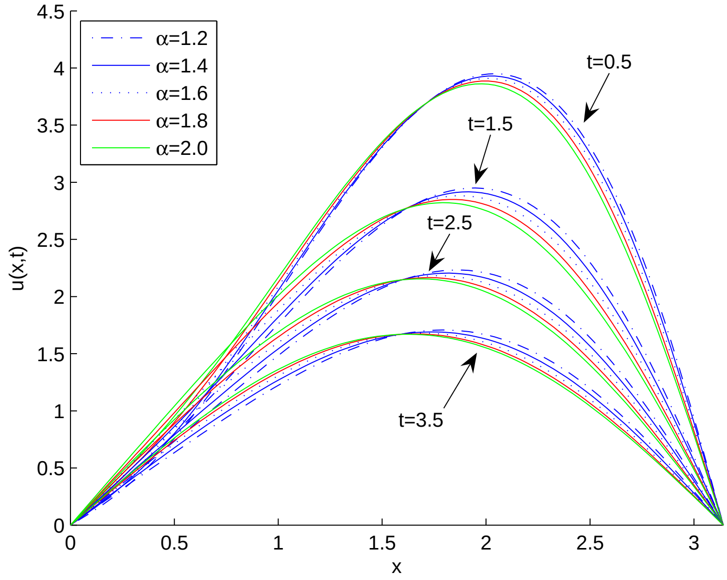

Fig. 2. The numerical approximation of $u(x,t)$ for the RFDE (35)-(37) with different values of $\alpha = 1.2, 1.4, 1.6, 1.8, 2.0$ when $t = 0.5, 1.5, 2.5, 3.5$.

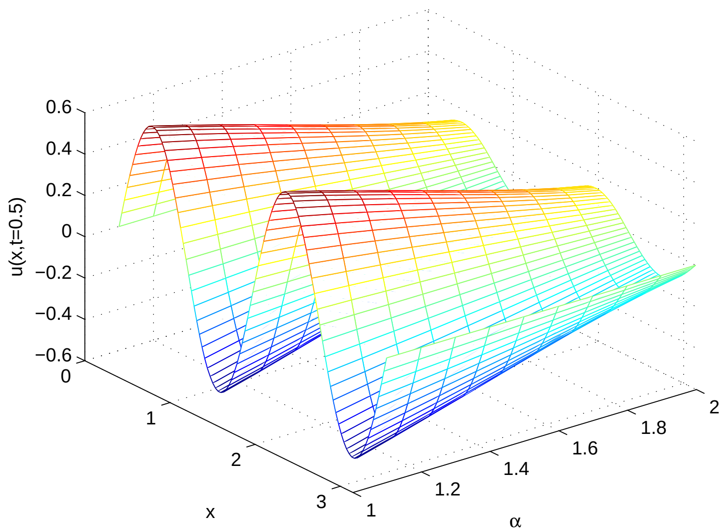

Fig. 3. The numerical approximation of $u(x,t)$ for the RFDE (38)-(40) when $t = 0.5$ and $K_\alpha = 0.25$.

Figure 3 presents the solution profiles of RFDE over space for $1 < \alpha \leq 2$ when $t = 0.5$. It can be observed that as α is decreased from 2 to 1 the amplitude of the sinusoidal solution behaviour is increased. Figure 4 displays the solution profiles of RFDE over space for $0 < t < 1$ when $\alpha = 2.0$ (left) and $\alpha = 1.5$ (right), respectively. We can see that the fractional diffusion ($\alpha = 1.5$) is slower than the standard diffusion ($\alpha = 2.0$). From Figures 1-4, we conclude that the

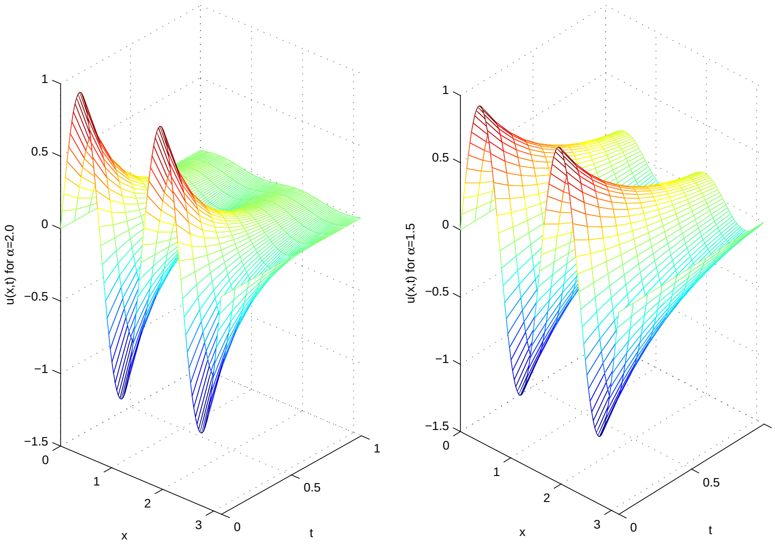

Fig. 4. A comparison of solutions for the RFDE (38)-(40) with $K_\alpha = 0.25$ when $\alpha = 2$ (left) and $\alpha = 1.5$ (right).

solution continuously depends on the Riesz space fractional derivatives.

5.2 Numerical examples of the RFADE

In this subsection, we present two examples of the RFADE on a finite domain $[0, \pi]$. Firstly, consider the following problem

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha u(x,t)}{\partial |x|^\alpha} + K_\beta \frac{\partial^\beta u(x,t)}{\partial |x|^\beta}, \quad 0 < x < \pi, \quad t > 0, \tag{41}$$

with the initial and boundary conditions given by

$$u(x,0) = x^2(\pi - x), \tag{42}$$
$$u(0,t) = u(\pi,t) = 0. \tag{43}$$

According to Section 4.1, the analytic solution of Eq.(41)-(43) is given by

$$u(x,t) = \sum_{n=1}^{\infty} [\frac{8}{n^3}(-1)^{n+1} - \frac{4}{n^3}] \sin(nx) \exp(-[K_\alpha (n^2)^{\frac{\alpha}{2}} + K_\beta (n^2)^{\frac{\beta}{2}}]t). \tag{44}$$

The analytical solution is compared with the numerical methods in Figure 5 for $t = 0.4$, $\alpha = 1.8$, $\beta = 0.4$, and $K_\alpha = K_\beta = 0.25$. It is seen that all three

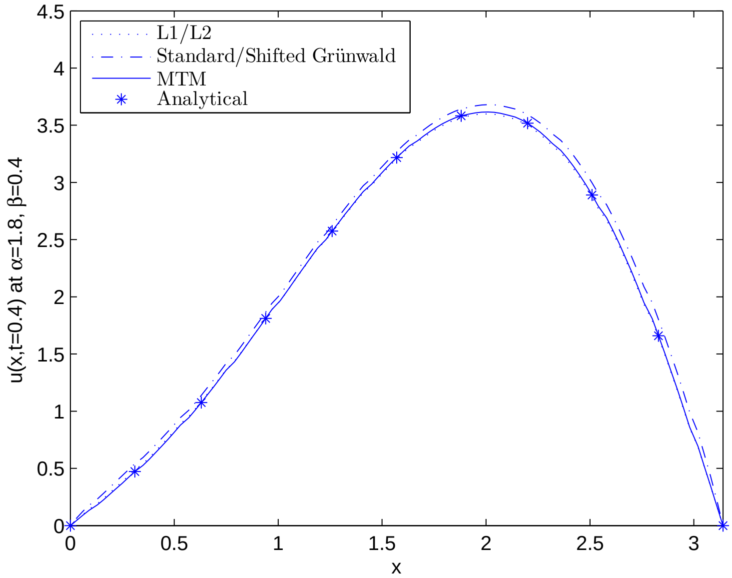

Fig. 5. Comparison of the numerical solutions with the analytic solution at $t = 0.4$ for the RFADE (41)-(43) with $\alpha = 1.8$, $\beta = 0.4$, and $K_\alpha = K_\beta = 0.25$.

numerical methods perform well. Based on the matrix method from Section 4.4, Figure 6 shows the solution profiles for different values of α at different times t, while Figure 7 shows the solution profiles for different values of β at different times t. In both figures, it can be seen that the process described by the RFADE is again slightly more skewed to the right than that modelled by the classical ADE ($\alpha = 2,\ \beta = 1$). To further demonstrate the impact of

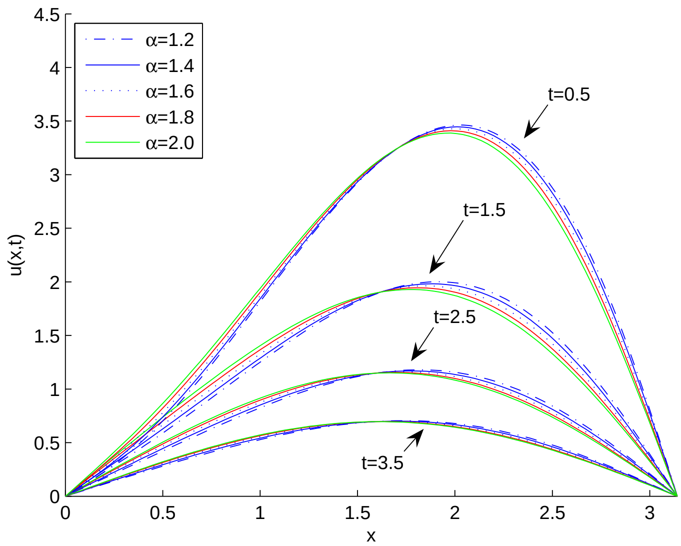

Fig. 6. The numerical approximation of $u(x,t)$ for the RFADE (41)-(43) with different values of $\alpha = 1.2, 1.4, 1.6, 1.8, 2.0$ when $\beta = 0.4$ and $t = 0.5, 1.5, 2.5, 3.5$.

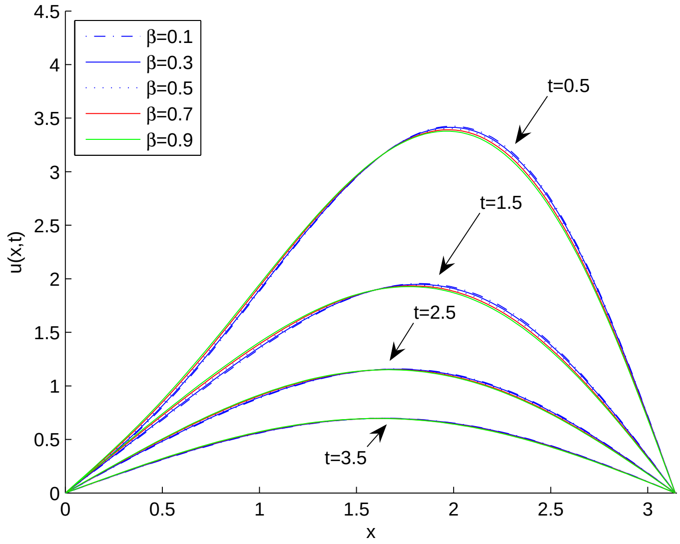

Fig. 7. The numerical approximation of $u(x,t)$ for the RFADE (41)-(43) with different values of $\beta = 0.1, 0.3, 0.5, 0.9$ when $\alpha = 1.8$ and $t = 0.5, 1.5, 2.5, 3.5$.

fractional order, another example of RFADE with a different initial condition is now considered:

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha u(x,t)}{\partial |x|^\alpha} + K_\beta \frac{\partial^\beta u(x,t)}{\partial |x|^\beta}, \quad 0 < x < \pi, \quad t > 0, \tag{45}$$

$$u(x,0) = \sin 4x, \tag{46}$$

$$u(0,t) = u(\pi,t) = 0. \tag{47}$$

Figures 8 and 9 displays the changes in the solution behaviours when α varies from 1 to 2 and β ranges from 0 to 1, respectively. In both figures, consistent with our observations for the RFDE in Section 5.1, we see that as α is decreased from 2 to 1 or β from 1 to 0 the amplitude of the sinusoidal solution behaviour is increased. In Figure 10, the solution profiles of RFADE over space for $0 < t < 1$ are displayed when $\alpha = 2.0$, $\beta = 1.0$ (left) and $\alpha = 1.5$, $\beta = 0.7$ (right), respectively. It can be observed that the fractional advection-dispersion process ($\alpha = 1.5$, $\beta = 0.7$) is slower than the classical advection-dispersion process ($\alpha = 2.0$, $\beta = 1.0$). Furthermore, from Figures 8-10, it is seen that the solution continuously depends on the Riesz space fractional derivatives. Finally, Figure 11 provides a comparison of the RFDE (38)-(40) and RFADE (45)-(47) with $K_\alpha = K_\beta = 0.25$ at time $t = 0.5$, where it can be observed that there is an offset when the fractional advection term is added to the fractional diffusion process.

Example 2 We consider the following equation

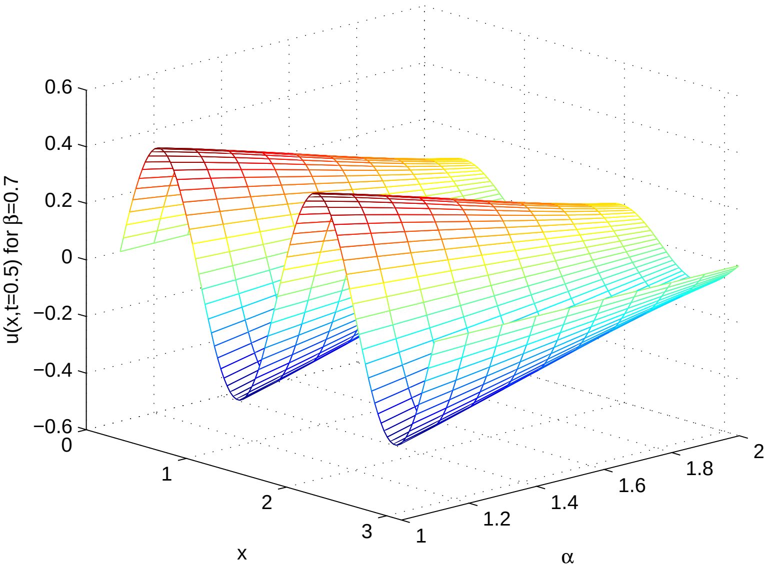

Fig. 8. The numerical approximation of $u(x,t)$ for the RFADE (45)-(47) when $\beta = 0.7$ and $t = 0.5$.

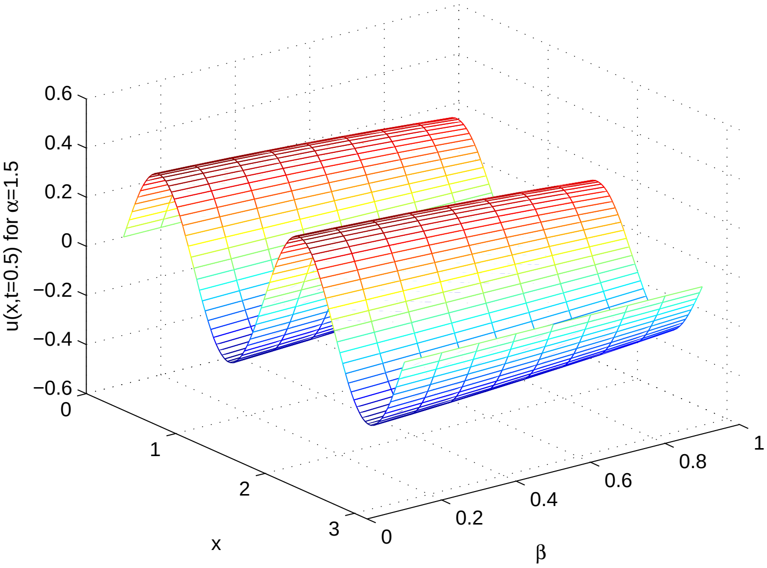

Fig. 9. The numerical approximation of $u(x,t)$ for the RFADE (45)-(47) when $\alpha = 1.5$ and $t = 0.5$.

$$\frac{\partial u(x,t)}{\partial t} = K_\alpha \frac{\partial^\alpha}{\partial |x|^\alpha} u(x,t) + K_\beta \frac{\partial^\beta}{\partial |x|^\beta} u(x,t) + f(x,t), 1 < x < 1,\ 0 < t \leq T, \tag{48}$$

with the initial and boundary conditions given by

$$u(x,0) = 0, \tag{49}$$

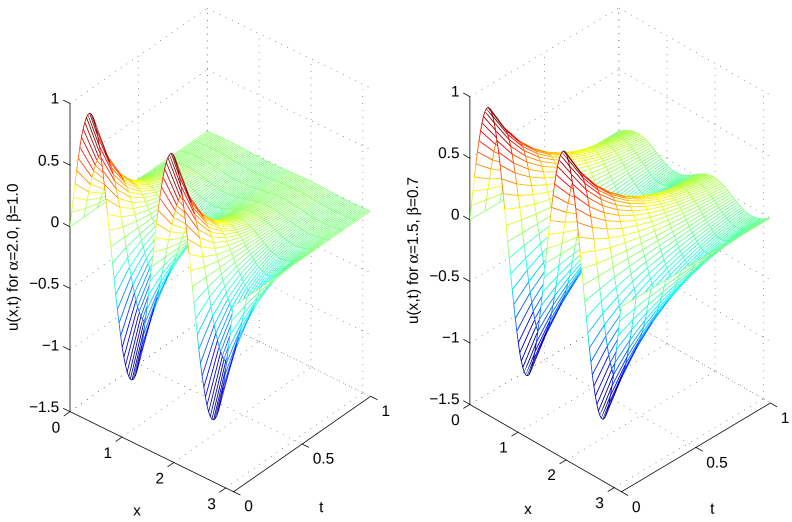

Fig. 10. A comparison of solutions for the RFADE (45)-(47) when $\alpha = 2.0$ and $\beta = 1.0$ (left) and $\alpha = 1.5$ and $\beta = 0.7$ (right).

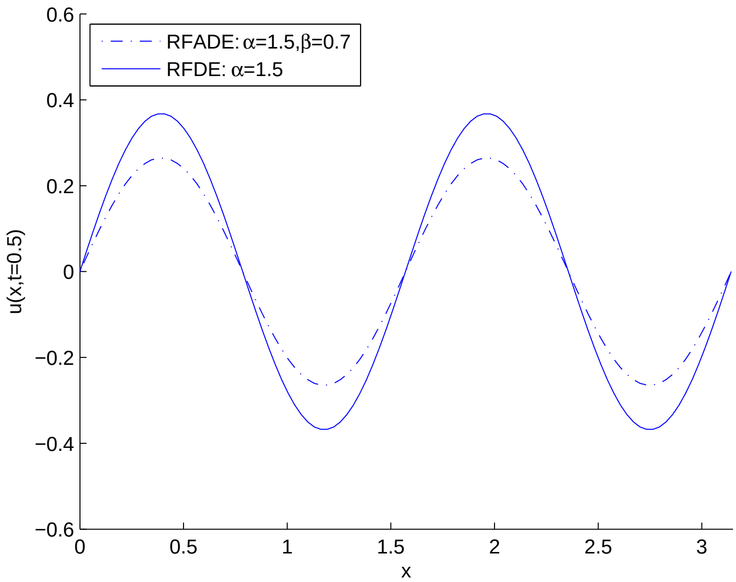

Fig. 11. Comparison of the RFDE (38)-(40) and RFADE (45)-(47) with $K_\alpha = K_\beta = 0.25$ at time $t = 0.5$.

$$u(0, t) = u(\pi, t) = 0, \tag{50}$$

where

$$
\begin{aligned}
f(x,t) =& \frac{K_\alpha t^\alpha e^{\beta t}}{2cos(\alpha\pi/2)}\left\{\frac{2}{\Gamma(3-\alpha)}[x^{2-\alpha}+(1-x)^{2-\alpha}] - \frac{12}{\Gamma(4-\alpha)}[x^{3-\alpha}+(1-x)^{3-\alpha}]\right. \\
&\left. + \frac{24}{\Gamma(5-\alpha)}[x^{4-\alpha}+(1-x)^{4-\alpha}]\right\} + \frac{K_\beta t^\alpha e^{\beta t}}{2cos(\beta\pi/2)}\left\{\frac{2}{\Gamma(3-\beta)}[x^{2-\beta}+(1-x)^{2-\beta}]\right. \\
&\left. - \frac{12}{\Gamma(4-\beta)}[x^{3-\beta}+(1-x)^{3-\beta}] + \frac{24}{\Gamma(5-\beta)}[x^{4-\beta}+(1-x)^{4-\beta}]\right\} \\
&+ t^{\alpha-1}e^{\beta t}(\alpha+\beta t)x^2(1-x)^2. \qquad (51)
\end{aligned}
$$

The exact solution of Eq.(48)-(50) is given by

$$u(x,t) = t^\alpha e^{\beta t} x^2(1-x)^2.$$

In this example, we take $\alpha = 1.7,\ \beta = 0.4,\ K_\alpha = K_\beta = 2.0,\ N = 100.$

6 CONCLUSIONS

In this paper, three effective numerical methods for solving the RFDE and RFADE on a finite domain with homogeneous Dirichlet boundary conditions have been described and demonstrated. They are the L1/L2-approximation method, the standard/shifted Grünwald method, and the matrix transform method. All three numerical methods perform well in approximating the analytic solution of the RFDE and RFADE derived using a spectral representation. The methods and techniques discussed in this paper can also be applied to solve other kinds of fractional partial differential equations, e.g., the modified fractional diffusion equation where $1 < \beta < \alpha \leq 2$.

Table 2
Maximum errors for 3 methods

$h = 1/N$	L_2 approximation	Matrix transform	Shifted Grünwald
1/50	1.8144E-2	3.2649E-2	2.8191E-3
1/100	9.4917E-3	3.2901E-2	1.5093E-3
1/200	4.8584E-3	3.2961E-2	7.7821E-4
1/400	2.4586E-3	overstack	3.9459E-4

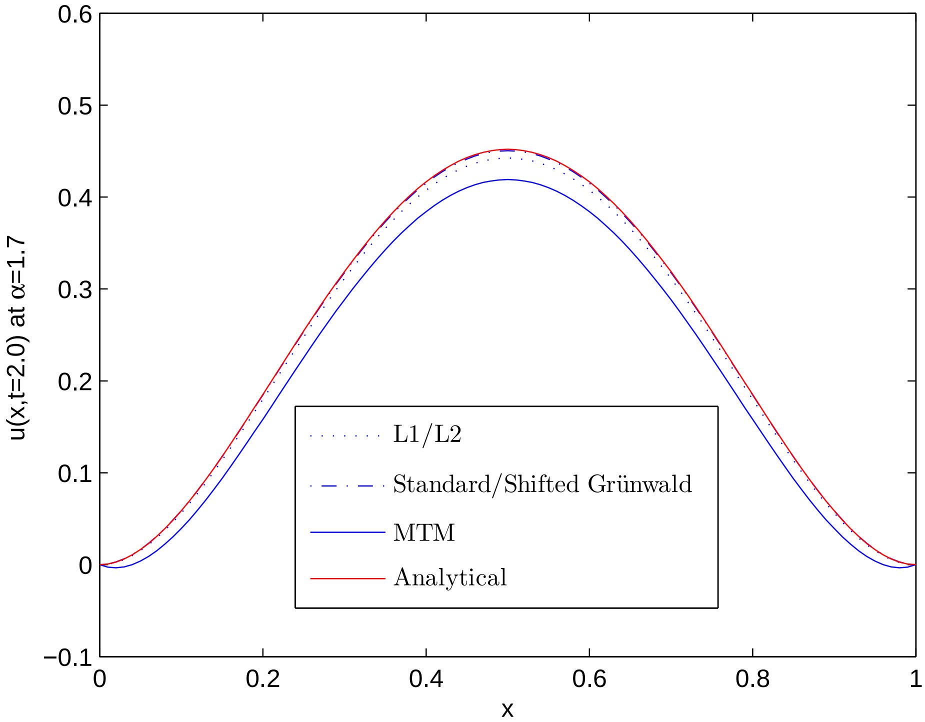

Fig. 12. A comparison of exact solution and three numerical solutions.

References

[1] Barkai E, Metzler R, Klafter J. From continuous time random walks to the fractional Fokker-Planck equation. *Physical Review E* 2000; **61**(1):132–138.

[2] Benson DA, Wheatcraft SW, Meerschaert MM. Application of a fractional advection-dispersion equation. *Water Resources Research* 2000; **36**(6):1403–1412.

[3] Benson DA, Wheatcraft SW, Meerschaert MM. The fractional-order governing equation of Lévy motion. *Water Resources Research* 2000; **36**(6):1413–1423.

[4] Bhatia SK, Liu F, Arvind G. Effect of pore blockage on adsorption isotherms and dynamics: Anomalous adsorption of iodine on activated carbon. *Langmuir* 2000; **16**(8):4001–4008.

[5] Brenan KE, Campbell SL, Petzold LR. *Numerical Solution of Initial-Value Problems in Differential-Algebraic Equations*. North-Holland, New York, 1989.

[6] Ciesielski M, Leszczynski J. Numerical Solutions of a Boundary Value Problem for the Anomalous Diffusion Equation with the Riesz Fractional Derivative. *Proceeding of the 16th International Conference on Computer Methods in Mechanics* Czestochowa, Poland, 2005.

[7] Gear CW. The automatic integration of ordinary differential equations, Comm. *ACM* 1971; **4**(3):176–179.

[8] Gorenflo R, Mainardi F. Random walk models for space-fractional diffusion processes. *Fractional Calculus and Applied Analysis* 1998; **1**(2):167–191.

[9] Gorenflo R, Mainardi F, Scalas E, Raberto M. Fractional calculus and continuous-time finance. III. The diffusion limit. *Mathematical finance (Konstanz, 2000)* 2001; page 171180.

[10] Hilfer R. Fractional diffusion based on Riemann-Liouville fractional derivatives. *J. Phys. Chem. B* 2000. **104**:3914-3917.

[11] Huang F, Liu F. The fundamental solution of the space-time fractional advection-dispersion equation. *J. Appl. Math.& Computing* 2005; **18**(1-2):339–350.

[12] Ilić M, Liu F, Turner I, Anh V. Numerical approximation of a fractional-in-space diffusion equation. *Fractional Calculus and Applied Analysis* 2005; **8**(3):323–341.

[13] Ilić M, Liu F, Turner I, Anh V. Numerical approximation of a fractional-in-space diffusion equation (II) — with nonhomogeneous boundary conditions. *Fractional Calculus and Applied Analysis* 2006; **9**(4):333–349.

[14] Liu F. *Numerical analysis of semiconductor device equations in two and three dimensions.* Ph.D. Thesis, Trinity College, Dublin, Ireland, 1991.

[15] Liu F, Anh V, Turner I. Numerical solution of the space fractional Fokker-Planck equation. *Journal of Computational and Applied Mathematics* 2004; **166**(1):209–219.

[16] Liu F, Anh V, Turner I, Zhuang P. Time fractional advection-dispersion equation. *J. Appl. Math. Computing* 2003; **13**(1-2):233–246.

[17] Liu F, Bhatia SK. Computationally efficient solution techniques for adsorption problems involving steep gradients in bidisperse particles. *Computers & Chemical Engineering* 1999; **23**:933–943.

[18] Liu F, Bhatia SK, Abarzhi II. Numerical solution of hyperbolic models of transport in bidisperse solids. *Computers & Chemical Engineering* 2000; **24**(8):1981–1995.

[19] Liu F, Bhatia SK. Solution techniques for transport problems involving steep concentration gradients: Application to noncatalytic fluid solid reactions. *Computers & Chemical Engineering* 2001; **25**(9-10):1159–1168.

[20] Liu F, Bhatia SK. Application of Petrov-Galerkin methods to transient boundary value problems in chemical engineering: Adsorption with steep gradients in bidisperse solids. *Chemical Engineering Science* 2001; **56**(12):3727–3735.

[21] Liu F, Turner I, Anh V. An unstructured mesh finite volume method for modelling saltwater intrusion into coastal aquifers. *The Korean Journal of Computational & Applied Mathematics* 2002; **9**(2):391–407.

[22] Liu F, Turner I, Anh V, Su N. A two-dimensional finite volume method for transient simulation of time-, scale- and density-dependent transport in heterogeneous aquifer systems. *J. Appl. Math. Comp* 2003; **11**:215–241.

[23] Liu Q, Liu F, Turner I, Anh V. Approximation of the Lévy-Feller advection-dispersion process by random walk and finite difference method. *J. Phys. Comp.* 2007; **222**(1):57–70.

[24] Mainardi F, Luchko Y, Pagnini G. The fundamental solution of the space-time fractional diffusion equation. *Fractional Calculus and Applied Analysis* 2001. **4**(2):153-192.

[25] Meerschaert MM, Scheffler HP, Tadjeran C. Finite difference methods for two-dimensional fractional dispersion equation. *Journal of Computational Physics* 2006. *211*(1):249-261.

[26] Meerschaert MM, Tadjeran C. Finite difference approximations for fractional advection-dispersion flow equations. *Journal of Computational and Applied Mathematics* 2004; **172**:65–77.

[27] Meerschaert MM, Tadjeran C. Finite difference approximations for two-sided space-fractional partial differential equations. *Applied Numerical Mathematics* 2006; **56**(1):80–90.

[28] Metzler R, Klafter J. Boundary value problems for fractional diffusion equations. *Physica A: Statistical Mechanics and its Applications* 2000; **278**(1-2):107–125.

[29] Metzler R, Klafter J. The random walk's guide to anomalous diffusion: a fractional dynamics approach. *Physics Reports* 2000; **339**(1):1–77.

[30] Miller KS, Ross B. *An Introduction to the Fractional Calculus and Fractional Differential Equations.* Wiley: 1993.

[31] Momani S, Odibat Z. Numerical solutions of the space-time fractional advection-dispersion equation. *J. Appl. Math. Comput* 2007; in press.

[32] Oldham KB, Spanier J. *The Fractional Calculus.* Academic Press: New York, 1974.

[33] Podlubny I. *Fractional Differential Equations.* Academic Press: New York, 1999.

[34] Raberto M, Scalas E, Mainardi F. Waiting-times and returns in high-frequency financial data: An empirical study. *Physica A: Statistical Mechanics and its Applications* 2002; **314**(1-4):749–755.

[35] Saichev AI, Zaslavsky GM. Fractional kinetic equations: solutions and applications. *Chaos* 1997; **7**(4):753–764.

[36] Samko SG, Kilbas AA, Marichev OI. *Fractional Integrals and Derivatives: Theory and Applications*. Gordon and Breach Science Publishers: Amsterdam, 1993.

[37] Scalas E, Gorenflo R, Mainardi F. Fractional calculus and continuous-time finance. *Physica A: Statistical Mechanics and its Applications* 2000; **284**(1-4):376–384.

[38] Shen S, Liu F, Anh V, Turner I. The fundamental solution and numerical solution of the Riesz fractional advection-dispersion equation. *IMA Journal of Applied Mathematics* 2008 **73**(6):850-872.

[39] Tocci MD, Kelley CT. Accurate and economical solution of the pressure-head from of Richards' equation by the method of lines. *Water resource* 1997; **20**(1):1–14.

[40] Wyss W. The fractional Black-Scholes equation. *Fractional Calculus Appl. Anal* 2000; **3**:51–61.

[41] Yuste SB, Acedo L, Lindenberg K. Reaction front in an A + B –> C reaction-subdiffusion process. *Physical Review E* 2004; **69**(3):036126.

[42] Yuste SB, Lindenberg K. Subdiffusion-limited A + A reactions. *Physical Review Letters* 2001; **87**(11):118301.

[43] Zaslavsky GM. Chaos, fractional kinetics, and anomalous transport. *Physics Reports* 2002; **371**(6):461–580.