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Analysis of a discrete non-Markovian random walk approximation for the time fractional diffusion equation

F. Liu[*] [†] S. Shen[*] V. Anh[†] I. Turner[†]

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Abstract

The time fractional diffusion equation (TFDE) is obtained from the standard diffusion equation by replacing the first-order time derivative with a fractional derivative of order in (0,1). In this work, an explicit finite-difference scheme for TFDE is presented. Discrete models of a non-Markovian random walk are generated for simulating random processes whose spatial probability density evolves in time according to this fractional diffusion equation. We derive the scaling restriction of the stability and convergence of the discrete non-Markovian random

[*]School of Mathematical Sciences, Xiamen University, Xiamen 361005, China. mailto:fwliu@xmu.edu.cn

[†]School of Mathematical Sciences, Queensland University of Technology, G.P.O. Box 2434, Brisbane, Queensland 4001, Australia. mailto:f.liu@qut.edu.au

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walk approximation for TFDE in a bounded domain. Finally, some numerical examples are presented to show the application of the present technique.

Contents

1 Introduction

Increasingly many authors from various fields of science and engineering deal with dynamical systems described by fractional-order differential equations [9]. Fractional-order differential equations provide a powerful instrument for the description of memory and hereditary properties of different substances. Diffusion equations that use time fractional derivatives are attractive because they describe a wealth of non-Markovian random walks.

Time fractional diffusion equations have recently been treated by some. Typically, the solution is given in closed form in terms of Fox functions [13].

Schneider and Wyss [10] considered the time fractional diffusion and wave equations and derived the corresponding Green functions in closed form for arbitrary space dimensions in terms of Fox functions. Gorenflo et al. [2] used similarity methods and Laplace transforms to obtain the scale invariant solution of the time fractional diffusion wave equation in terms of the Wright function. However, an explicit representation of the Green functions for the problem in a half-space is difficult to determine, except in the special cases of a first-order time derivative in arbitrary dimension n, or $n = 1$ with arbitrary fractional-order time derivative. Huang and Liu [4] considered the time-fractional diffusion equations in an n-dimensional whole-space and half-space. They investigated the explicit relationships between the problems in whole-space with the corresponding problems in half-space by the Fourier–Laplace transform. Liu et al. [5] considered time fractional advection dispersion equation and derived the complete solution.

The most significant advantage of fractional order models in comparison with integer order models is based on its important fundamental physical considerations. However, because of the absence of appropriate mathematical methods, fractional order dynamical systems were studied only marginally in theory and practice of control systems. Numerical methods and theoretical analysis of fractional differential equations are very difficult tasks [6, 7].

Time fractional diffusion and wave equations have been derived by considering continuous time random walk (CTRW) problems, which generally involve non-Markovian processes, and via diffusion in fractal media. Diffusion equations with fractional spatial derivative are used for studying Lévy stable processes. The physical interpretation of the fractional derivative in both cases is that it represents a degree of memory in the diffusing material.

Here, numerical methods of the time fractional diffusion equation (TFDE) are considered. TFDE has been investigated by several authors for different purposes [3, 13]. Gorenflo et al. [3] adopted a suitable finite-difference scheme and generated a discrete random walk approach. From a physical view point, this generalized diffusion equation is obtained from a fractional Fick law that describes transport processes with long memory. The fundamental solution of the TFDE is interpreted as a probability density of a self-similar non-Markovian stochastic process related to a phenomenon of slow anomalous diffusion [14]. We use an effective explicit finite-difference scheme [11] for TFDE, and generate discrete models of random walk suitable for simulating random variables whose spatial probability density evolves in time according to this fractional diffusion equation. Subsequently, the conditions for the stability and convergence of the explicit finite-difference scheme for TFDE in a bounded domain are derived. Some numerical examples are presented. The results show that for time fractional derivatives of order $\alpha \in (0,1)$, the system exhibits diffusion behaviors. The techniques can be applied to deal with fractional-order dynamical systems and controllers.

2 The discrete non-Markovian random walk approximation

Consider the time fractional diffusion equation

$$ {}_tD_*^\alpha u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t)\,, \quad 0<\alpha<1\,, \quad x\in\mathbb{R}\,, \quad t\in\mathbb{R}_0^+\,, \tag{1} $$

where ${}_tD_*^\alpha$ denotes the time fractional derivative intended in the *Caputo* sense:

$$ {}_tD_*^\alpha u(x,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \left[\frac{\partial u(x,\tau)}{\partial \tau}\right] \frac{d\tau}{(t-\tau)^\alpha}\,, \quad 0<\alpha<1\,. $$

In the case $\alpha = 1$, the standard diffusion (heat equation) is recovered. In the case $0<\alpha<1$, we have to consider the previous time levels (non-Markovian process).

Now discretize space and time at grid points and time instants:

$$ x_j = jh\,, \quad h>0\,, \quad j = 0, \pm 1, \pm 2, \ldots\,; $$

$$t_n = n\tau\,, \quad \tau > 0\,, \quad n = 0, 1, 2, \ldots, N\,,$$

where h and τ are space and time steps, respectively. The dependent variable u is then discretized (after multiplication of (1) by the spatial mesh width h) by introducing $y_j(t_n)$ as the intended approximation to

$$\int_{x_j-h/2}^{x_j+h/2} u(x,t_n)\,dx \approx hu(x_j,t_n)\,.$$

With the quantities $y_j(t_n)$ so intended, we replace the time fractional diffusion equation (1), by the finite-difference equation

$$ {}_tD_*^\alpha y_j(t_{n+1}) = \frac{y_{j+1}(t_n) - 2y_j(t_n) + y_{j-1}(t_n)}{h^2}\,, \quad 0 < \alpha \leq 1\,. \tag{2}$$

As usual, we adopt a second-order central difference in space at level $t = t_n$ for approximating the second-order space derivative. The time fractional diffusion term is approximated by

$$\begin{aligned} {}_tD_*^\alpha y_j(t_{n+1}) &= \frac{1}{\Gamma(1-\alpha)} \sum_{i=0}^{n} \int_{i\tau}^{(i+1)\tau} \frac{y_j'(t_{n+1}-r)}{r^\alpha}\,dr \\ &= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \Big\{ \big[y_j(t_{n+1}) - y_j(t_n)\big] \\ &\quad + \sum_{i=1}^{n} \big[y_j(t_{n+1-i}) - y_j(t_{n-i})\big]\big[(i+1)^{(1-\alpha)} - i^{(1-\alpha)}\big] \Big\}. \end{aligned} \tag{3}$$

Thus, the discrete form of the equation (1) is

$$\begin{aligned} &\big[y_j(t_{n+1}) - y_j(t_n)\big] + \sum_{i=1}^{n} \big[y_j(t_{n+1-i}) - y_j(t_{n-i})\big]\big[(i+1)^{(1-\alpha)} - i^{(1-\alpha)}\big] \\ &= \mu\Gamma(2-\alpha)\big[y_{j+1}(t_n) - 2y_j(t_n) + y_{j-1}(t_n)\big]\,, \end{aligned} \tag{4}$$

where $\mu := \tau^\alpha/h^2$. Rearranging, we obtain

$$y_j(t_{n+1}) \;=\; \mu\Gamma(2-\alpha)y_{j+1}(t_n) + \big[2 - 2^{1-\alpha} - 2\mu\Gamma(2-\alpha)\big]y_j(t_n)$$

$$\begin{aligned}&+\mu\Gamma(2-\alpha)y_{j-1}(t_n)+\big[2\cdot 2^{1-\alpha}-1-3^{1-\alpha}\big]y_j(t_{n-1})\\&+\big[2\cdot 3^{1-\alpha}-2^{1-\alpha}-4^{1-\alpha}\big]y_j(t_{n-2})\\&+\cdots+\big[2\cdot n^{1-\alpha}-(n-1)^{1-\alpha}-(n+1)^{1-\alpha}\big]y_j(t_1)\\&+\big[(n+1)^{1-\alpha}-n^{1-\alpha}\big]y_j(t_0)\,.\end{aligned}\tag{5}$$

Introduce the coefficients

$$\begin{aligned}c_k &= 2k^{1-\alpha}-(k-1)^{1-\alpha}-(k+1)^{1-\alpha}\,,\quad k\geq 1\,,\\ b_n &= (n+1)^{1-\alpha}-n^{1-\alpha}\,,\quad n\geq 0\,.\end{aligned}\tag{6}$$

Then write equation (5) in the following discrete non-Markovian random walk approximation, hereafter referred to as DNMRWA:

$$\begin{aligned}y_j(t_{n+1}) &= b_n y_j(t_0)+\sum_{k=1}^{n} c_k y_j(t_{n+1-k})\\&\quad+\mu\Gamma(2-\alpha)\big[y_{j+1}(t_n)-2y_j(t_n)+y_{j-1}(t_n)\big]\,.\end{aligned}\tag{7}$$

In particular,

for $n=0$,

$$y_j(t_1)=y_j(t_0)+\mu\Gamma(2-\alpha)\big[y_{j+1}(t_0)-2y_j(t_0)+y_{j-1}(t_0)\big];$$

for $n=1$,

$$y_j(t_2)=b_1y_j(t_0)+\big[c_1-2\mu\Gamma(2-\alpha)\big]y_j(t_1)+\mu\Gamma(2-\alpha)\big[y_{j+1}(t_1)+y_{j-1}(t_1)\big];$$

for $n\geq 2$,

$$\begin{aligned}y_j(t_{n+1}) &= b_n y_j(t_0)+\sum_{k=2}^{n} c_k y_j(t_{n+1-k})+\big[c_1-2\mu\Gamma(2-\alpha)\big]y_j(t_n)\\&\quad+\mu\Gamma(2-\alpha)\big[y_{j+1}(t_n)+y_{j-1}(t_n)\big].\end{aligned}$$

For $0 < \alpha < 1$, the coefficients (6) possess the properties

$$
\begin{aligned}
&1 = b_0 > b_1 > b_2 > b_2 > \cdots \to 0\,,\\
&c_k = b_{k-1} - b_k\,, \quad \sum_{k=1}^{n} c_k = 1 + n^{1-\alpha} - (n+1)^{1-\alpha}\,,\\
&\sum_{k=1}^{\infty} c_k = 1\,, \quad 1 > 2 - 2^{1-\alpha} = c_1 > c_2 > c_3 > \cdots \to 0\,.
\end{aligned} \tag{8}
$$

Two propositions follow from equation (7), see [8] for further details.

Proposition 1 *The term $y_j(t_{n+1})$ preserves non-negativity if all coefficients are non-negative.*

Hence, we require that the coefficient of the term $y_j(t_n)$ be non-negative, that is,

$$
0 < \mu = \frac{\tau^\alpha}{h^2} \le \frac{1}{\Gamma(2-\alpha)}\left(1 - \frac{1}{2^\alpha}\right). \tag{9}
$$

The following result can be proved using mathematical induction [8].

Proposition 2 DNMRWA *is conservative, that is,*

$$
\sum_{j=-\infty}^{+\infty} |y_j(t_0)| < \infty \Rightarrow \sum_{j=-\infty}^{+\infty} y_j(t_n) = \sum_{j=-\infty}^{+\infty} y_j(t_0)\,, \quad n \in \mathbb{N}\,. \tag{10}
$$

Remark 3 Non-negativity preservation and conservation implies that our scheme can be interpreted as a redistribution scheme of clumps $y_j(t_n)$ [3].

3 Stability analysis of DNMRWA

We now discuss the stability of the DNMRWA for TFDE in a bounded domain $[0, L]$ with the following initial and boundary conditions:

$$\begin{aligned} u(0,t) &= u(L,t) = 0\,, \quad t \ge 0\,, \\ u(x,0) &= f(x)\,, \quad 0 < x < L\,. \end{aligned} \tag{11}$$

For the given initial and boundary conditions (11), equation (7) is expressed in matrix form as

$$\begin{cases} \mathbf{Y_1} = \mathbf{B}\mathbf{Y_0}\,, & n = 0\,, \\ \mathbf{Y_{n+1}} = \mathbf{A}\mathbf{Y_n} + c_2\mathbf{Y_{n-1}} + c_3\mathbf{Y_{n-2}} + \cdots + c_n\mathbf{Y_1} + b_n\mathbf{Y_0}\,, & n \ge 1\,, \end{cases} \tag{12}$$

where

$$\mathbf{Y_n} = \begin{bmatrix} y_{1,n} \\ y_{2,n} \\ \vdots \\ y_{m-1,n} \end{bmatrix}, \quad \mathbf{A} = \begin{bmatrix} c_1 - 2\eta & \eta & & & \\ \eta & c_1 - 2\eta & \eta & & \\ & & \ddots & \ddots & \eta \\ & & & \eta & c_1 - 2\eta \end{bmatrix},$$

$$\mathbf{B} = \begin{bmatrix} 1 - 2\eta & \eta & & & \\ \eta & 1 - 2\eta & \eta & & \\ & & \ddots & \ddots & \eta \\ & & & \eta & 1 - 2\eta \end{bmatrix}.$$

The matrices $\mathbf{A}$ and $\mathbf{B}$ are both tridiagonal of order $m - 1$.

We now analyse the stability via mathematical induction. First assume that the matrix $\mathbf{B}$ satisfies $\|\mathbf{B}\|_\infty \le 1$.

Next, when $n = 1$, we have $Y_1 = BY_0$; thus

$$\|\mathbf{Y_1}\|_\infty \le \|\mathbf{B}\|_\infty \cdot \|\mathbf{Y_0}\|_\infty \le \|\mathbf{Y_0}\|_\infty\,.$$

Now assume that $\|\mathbf{Y_k}\|_\infty \le \|\mathbf{Y_0}\|_\infty$ holds for $n \le k$. When $n = k+1$, we have

$$\begin{aligned} \|Y_{k+1}\|_\infty &= \|AY_k + c_2 Y_{k-1} + c_3 Y_{k-2} + \cdots + c_k Y_1 + b_k Y_0\|_\infty \\ &\le \big[\|A\|_\infty + c_2 + c_3 + \cdots + c_k + b_k\big] \cdot \|Y_0\|_\infty \,. \end{aligned}$$

If we assume that $\mu \le (1-2^{-\alpha})/\Gamma(2-\alpha)$, that is, $c_1 \ge 2\eta$, then

$$\|A\|_\infty + c_2 + c_3 + \cdots + c_k + b_k = \eta + c_1 - 2\eta + \eta + \textstyle\sum_{i=2}^{k} c_i + b_k = 1 \,.$$

Thus, $\|\mathbf{Y_{k+1}}\|_\infty \le \|\mathbf{Y_0}\|_\infty$.

Also notice that when $\mu \le (1-2^{-\alpha})/\Gamma(2-\alpha)$, that is, $c_1 \ge 2\eta$, the matrix $\mathbf{B}$ satisfies $\|\mathbf{B}\|_\infty \le 1$. We therefore conclude that, if $\mu \le (1-2^{-\alpha})/\Gamma(2-\alpha$ for any natural number n, then $\|\mathbf{Y_n}\|_\infty \le \|\mathbf{Y_0}\|_\infty$. According to the Lax–Richtmer definition of stability [12], the following theorem is obtained:

Theorem 4 *When $\mu \le (1-2^{-\alpha})/\Gamma(2-\alpha)$, the* DNMRWA *(7) for the* TFDE *in a bounded domain is stable.*

4 Convergence analysis of DNMRWA

The convergence of the solution of an approximating set of difference equations to the solution of a TFDE can be investigated directly by deriving DNMRWA for the discretization error e. Denote the exact solution of the TFDA by U and the approximation solution of the DNMRWA by y . Then $e = U - y$. We have adopted the DNMRWA (7) approximation to (1) with initial and boundary conditions (11).

At the mesh points,

$$y_{j,n} = U_{j,n} - e_{j,n} \,, \quad y_{j,n+1} = U_{j,n+1} - e_{j,n+1} \,, \quad \ldots \,.$$

It can be shown that the error vectors satisfy

$$\begin{cases} \mathbf{E_{n+1}} & = & \mathbf{A}\mathbf{E_n} + c_2\mathbf{E_{n-1}} + c_3\mathbf{E_{n-2}} + \cdots + c_n\mathbf{E_1} + \mathbf{M}\,, \quad n = 0, 1, \ldots\,, \\ \mathbf{E_0} & = & 0\,, \end{cases} \tag{13}$$

where

$$\mathbf{E_n} = \begin{bmatrix} e_{1,n} \\ e_{2,n} \\ \vdots \\ e_{m-1,n} \end{bmatrix}, \quad \mathbf{M} = \begin{bmatrix} \tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right) \\ \tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right) \\ \vdots \\ \tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right) \end{bmatrix}.$$

Now we use mathematical induction to analyse the convergence. We intend to show that

$$\|\mathbf{E_n}\|_\infty \leq n\tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right).$$

When $n = 1$, we have $\|E_1\|_\infty = \|M\|_\infty = \tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right)$. We now assume that the above inequality holds for $n \leq k$. Then, when $n = k+1$,

$$\begin{aligned} \|E_{k+1}\|_\infty &= \|AE_k + c_2E_{k-1} + c_3E_{k-2} + \cdots + c_kE_1 + M\|_\infty \\ &\leq \left[\|A\|_\infty\cdot k + c_2\cdot(k-1) + \cdots + c_{k-1}\cdot 2 + c_k + 1\right]\cdot\|M\|_\infty. \end{aligned}$$

If we assume that $\mu \leq (1-2^{-\alpha})/\Gamma(2-\alpha)$, that is, $c_1 \geq 2\eta$, then $\|A\|_\infty = c_1$. Thus,

$$\begin{aligned} \|E_{k+1}\|_\infty &\leq [c_1\cdot k + c_2\cdot(k-1) + \cdots + c_{k-1}\cdot 2 + c_k + 1]\cdot\|M\|_\infty \\ &\leq \left[k\cdot\sum_{i=1}^{k} c_i + 1\right]\cdot\|M\|_\infty \\ &\leq (k+1)\cdot\tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right). \end{aligned}$$

As a result, if $\mu \leq (1-2^{-\alpha})/\Gamma(2-\alpha)$ for any natural number n, then $\|\mathbf{E_n}\|_\infty \leq n\tau^\alpha\Gamma(2-\alpha)\cdot\mathcal{O}\left(\tau+h^2\right)$. Note that $n\tau \leq T$ is finite, $n\tau^\alpha\Gamma(2-\alpha)$ is also finite. So when $\tau \to 0$, $h \to 0$, we have $\|\mathbf{E_n}\|_\infty \to 0$, thus $|e_{j,n}| \to 0$.

The following result therefore holds:

Theorem 5 *Let U be the exact solution of the* TFDE *and y the approximate solution of the* DNMRWA*; then y converges to U as h and τ tend to zero when $\mu \leq (1-2^{-\alpha})/\Gamma(2-\alpha)$.*

Remark 6 We note that the condition for the convergence conforms with the condition for stability, and it is also the scaling restriction (9) for the random walk interpretation.

5 Numerical results

Consider the following time fractional diffusion equation

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{\partial^2 u(x,t)}{\partial x^2}\,, \quad 0 \leq x \leq 2\,, \quad t > 0\,, \tag{14}$$

with the initial and boundary conditions:

$$\begin{aligned} u(0,t) &= u(L,t) = 0\,, \quad t \geq 0\,, \\ u(x,0) &= f(x) = \begin{cases} 2x\,, & 0 \leq x \leq \frac{1}{2}\,, \\ \frac{4-2x}{3}\,, & \frac{1}{2} \leq x \leq 2\,. \end{cases} \end{aligned} \tag{15}$$

The function $f(x)$ represents the temperature distribution in a bar generated by a point heat source kept at the point $x = \frac{1}{2}$ for sufficiently long time.

By taking the finite sine transform and Laplace transform, the analytical solution for equation (14) with the initial and boundary conditions (15) is [1]

$$u(x,t) = \frac{2}{L} \sum_{n=1}^{\infty} E_\alpha(-a^2 n^2 t^\alpha) \sin(anx) \int_0^L f(r) \sin(anr)\, dr\,, \tag{16}$$

where $a = \pi/L$, $E_\alpha(z) = \sum_{k=0}^{\infty} z^k/\Gamma(\alpha k + 1)$ is the Mittag–Leffler function.

TABLE 1: The analytical solution, numerical solution and errors for TFDE at $t = 0.4$, $\alpha = 0.5$ with $h = 0.25$ and $\tau = 0.0004$

x_i	Exact	Numerical	Error
0.25	0.1114	0.1151	0.37E-02
0.50	0.1950	0.2048	0.97E-02
0.75	0.2360	0.2431	0.71E-02
1.00	0.2383	0.2404	0.20E-02
1.25	0.2018	0.2063	0.44E-02
1.50	0.1468	0.1497	0.28E-02
1.75	0.0773	0.0784	0.11E-02

TABLE 2: The analytical solution, numerical solution and errors for TFDE at $t = 0.4$ for $\alpha = 0.5$ with $h = 0.2$ and $\tau = 0.0001$

x_i	Exact	Numerical	Error
0.2	0.0905	0.0904	0.19E-03
0.4	0.1663	0.1677	0.14E-02
0.6	0.2168	0.2188	0.19E-02
0.8	0.2389	0.2356	0.83E-03
1.0	0.2383	0.2356	0.27E-02
1.2	0.2105	0.2115	0.99E-03
1.4	0.1709	0.1718	0.85E-03
1.6	0.1204	0.1207	0.31E-03
1.8	0.0622	0.0622	0.37E-04

The analytical solution, numerical solution (DNMRWA) and errors for TFDE at $t = 0.4$, $\alpha = 0.5$ with $h = 0.25$, $\tau = 0.0004$ and with $h = 0.2$ and $\tau = 0.0001$ are listed in Tables 1 and 2, respectively. Tables 1 and 2 show that the rate of convergence is $\mathcal{O}(\tau + h^2)$. Here

$$0 < \mu = \frac{\tau^\alpha}{h^2} \leq \frac{1}{\Gamma(2-\alpha)}\left(1 - \frac{1}{2^\alpha}\right) .$$

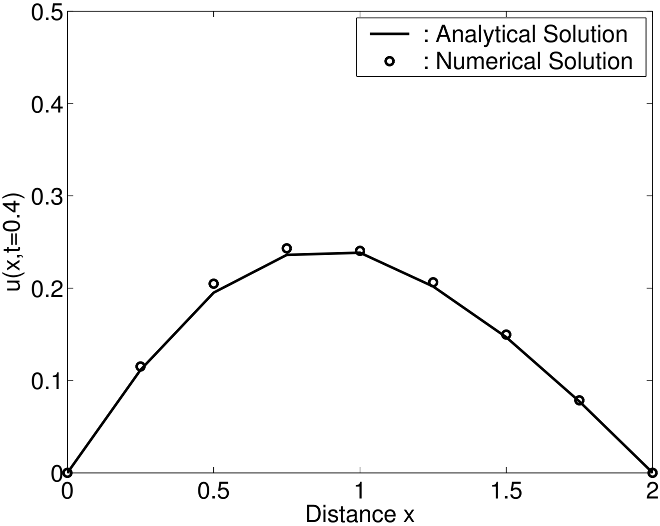
Now we present some results to demonstrate that the DNMRWA can be applied to simulate the behavior of the solution of a fractional diffusion equation as the order of the fractional derivative is changed. Such a numerical technique overcomes the problem of not being able to evaluate the analytical solution for $0 < \alpha \leq 1$ due to the nature of the Mittag–Leffler function.

Figure 1(a) shows the results of DNMRWA with $h = 0.25$, $\tau = 0.0004$ and the analytical solution for TFDE at $t = 0.4$ and $\alpha = 0.5$. It is apparent from Figure 1(a) that the numerical solution (DNMRWA) is in good agreement with the analytical solution. Figure 1(b) shows the evolution result using DNMRWA with $h = 0.25$, $\tau = 0.0004$ for $\alpha = 0.5$. From Figure 1(b), see that the $\alpha = 0.5$ order derivative system exhibits fast diffusion in the beginning and slow diffusion later.

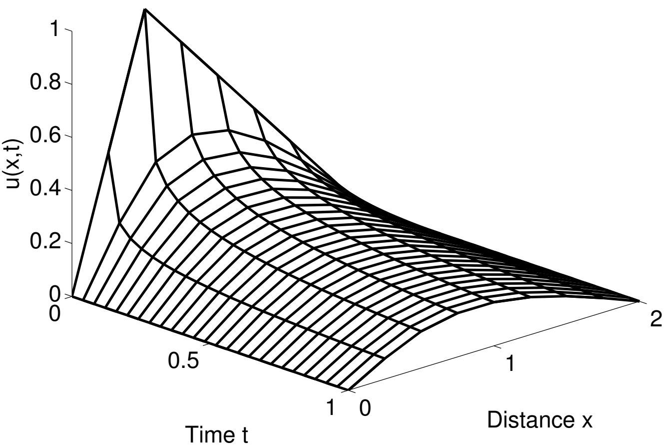
Figures 2(a) and 2(b) compare the response of the diffusion system for different real numbers $0 < \alpha \leq 1$ at $t = 0.4$ and different x, and at $x = 0.5$ and different t, respectively. Here h and τ satisfy the restriction (9). Figure 2 shows that DNMRWA can be applied to solve fractional-order dynamical systems.

6 Conclusions

The time fractional diffusion equation arises in a natural way when space-probability distributions evolve in time consistently with the phenomenon



(a)



(b)

FIGURE 1: (a) The analytical solution and the numerical solution at $t = 0.4$ for $\alpha = 0.5$; (b) Evolution of the initial state of the numerical solution ($\alpha = 0.5$)

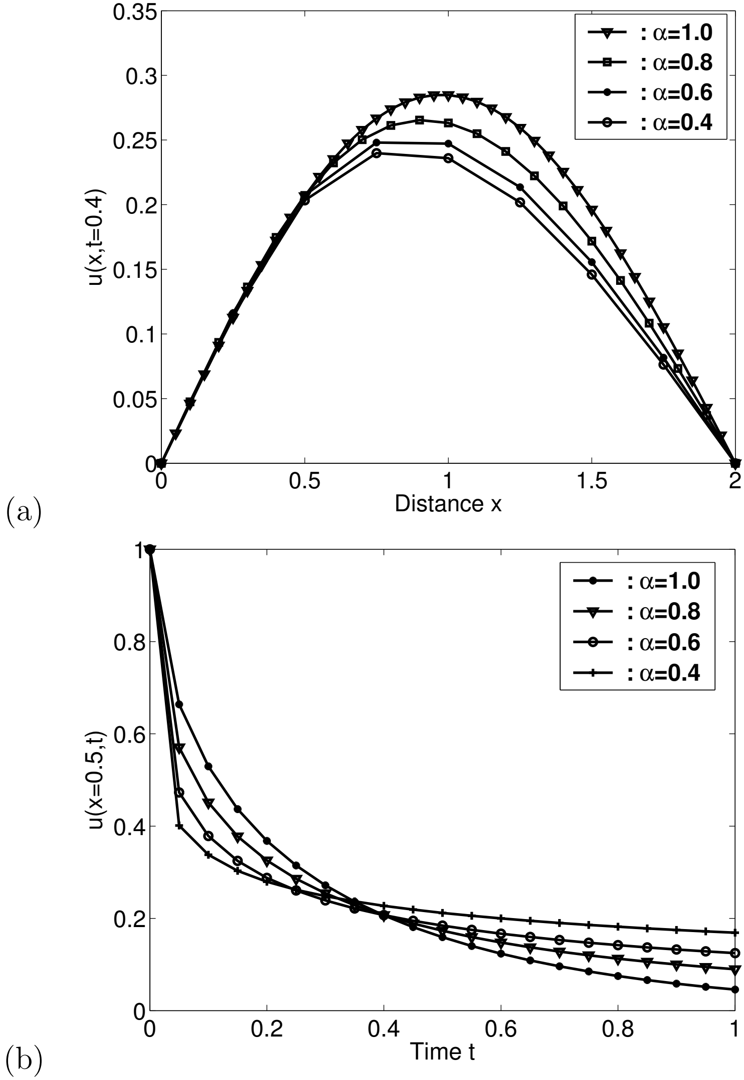


FIGURE 2: (a) Displacement at $t = 0.4$ as a function of x for various α; (b) Displacement at $x = 0.5$ as a function of t for various α.

of slow anomalous diffusion. In this paper we have provided DNMRWA for TFDE, and we generate discrete models of a random walk approach to this phenomenon. The DNMRWA possesses, with the scaling restriction (9) and simulating on a discrete space-time grid, the essential properties of the continuous process, namely, conservation and preservation of non-negativity. We also have proved that the scaling restriction is the condition for the stability and convergence of our scheme for TFDE in a bounded domain. The method can be applied to solve fractional-order dynamical systems.

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