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

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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 $\alpha \in (0, 1)$. In this work, an explicit finite-difference scheme for TFDE is presented. Discrete models of a non-Markovian random walk are generate for simulating random variables 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 walk approximation for TFDE in a bounded domain. Finally, some numerical examples are presented to show the application of the present technique.

Contents

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1 Introduction

A growing number of works by 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 walk.

Time fractional diffusion equations have recently been treated by a number of authors. 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 the similarity method and the method of Laplace transform 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 $\alpha = 1$ (i.e., the first-order time derivative) with arbitrary n, or $n = 1$ with arbitrary α (i.e., the fractional-order time derivative). Huang and Liu [4] considered the time-fractional diffusion equations in an n-dimensional whole-space and half-space. They investigate 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 the 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 analyse 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 problems(CTRW), which are in general non-Markovian processes, and via diffusion in fractal media. Space fractional diffusion equations with the fractional derivative on the spatial derivative are used for studying Markovian processes. The physical interpretation of the fractional derivative in both cases is that it represents a degree of memory in the diffusing material.

In this paper, numerical methods of the time fractional diffusion equation (TFDE) is 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 [**?**]. 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. 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

In this section the following time fractional diffusion equation is considered:

$$ {}_tD_*^{\alpha} u(x,t) = \frac{\partial^2}{\partial x^2} u(x,t), 0 < \alpha < 1, x \in \mathbf{R}, t \in R_0^+, \tag{1} $$

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

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

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

We now discretize space and time by grid points and time instants as follows:

$$ x_j = jh, h > 0, j = 0, \pm 1, \pm 2, \ldots; t_n = n\tau, \tau > 0, n = 0, 1, 2, \ldots, N $$

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

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

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

As usual, we have adopted a second-order central difference in space at level $t=t_n$ for approximating the second-order space derivative. The time fractional diffusion term can be approximated by the following scheme:

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

Thus, the discrete form of the equation (1) can be expressed as:

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

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

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

Introduce the coefficients c_k,b_n defined as follows

$$ \left\{ \begin{array}{lcll} c_k & = & 2k^{1-\alpha}-(k-1)^{1-\alpha}-(k+1)^{1-\alpha}\ , & k\ge 1, \\ b_n & = & (n+1)^{1-\alpha}-n^{1-\alpha}\ , & n\ge 0. \end{array} \right. \tag{6} $$

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

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

In particular,
for $n = 0$:

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

for $n = 1$:

$$y_j(t_2) = b_1 y_j(t_0) + [c_1 - 2\mu\Gamma(2-\alpha)]y_j(t_1) + \mu\Gamma(2-\alpha)[y_{j+1}(t_1) + y_{j-1}(t_1)];$$

and for $n \geq 2$:

$$y_j(t_{n+1}) = b_n y_j(t_0) + \sum_{k=2}^{n} c_k y_j(t_{n+1-k}) + [c_1 - 2\mu\Gamma(2-\alpha)]y_j(t_n)$$

$$+\mu\Gamma(2-\alpha)[y_{j+1}(t_n) + y_{j-1}(t_n)].$$

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

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

From equation (7), the following properties can be established, see [8] for further details.

Property 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, i.e.,

$$0 < \mu = \frac{\tau^\alpha}{h^2} \leq \frac{1}{\Gamma(2-\alpha)}(1 - \frac{1}{2^\alpha}). \quad (9)$$

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

Property 2: DNMRWA is conservative, i.e.,

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

Remark 1: Non-negativity preservation and conservativity implies that our scheme can be interpreted as a redistribution scheme of clumps $y_j(t_n)$ [3].

3 Stability analysis of DNMRWA

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

$$\left\{ \begin{array}{lcl} u(0,t) & = & u(L,t) = 0,\ t \geq 0, \\ u(x,0) & = & f(x),\ 0 < x < L. \end{array} \right. \tag{11}$$

For the given initial and boundary conditions (11), equation (7) can be expressed in matrix form:

$$\mathbf{V_{n+1}} = \mathbf{P V_n} \tag{12}$$

where $y_j(t_n) = y_{j,n}$, $\mu\Gamma(2-\alpha) = \eta$,

$$\mathbf{V_{n+1}} = \begin{bmatrix} \mathbf{Y_{n+1}} \\ \vdots \\ \mathbf{Y_3} \\ \mathbf{Y_2} \\ \mathbf{Y_1} \end{bmatrix}, \mathbf{P} = \begin{bmatrix} \mathbf{A} & c_2\mathbf{I_{m-1}} & c_3\mathbf{I_{m-1}} & \cdots & c_n\mathbf{I_{m-1}} & b_n\mathbf{I_{m-1}} \\ & \ddots & \ddots & \vdots & \vdots & \vdots \\ & & & & c_2\mathbf{I_{m-1}} & b_2\mathbf{I_{m-1}} \\ & & & & \mathbf{A} & b_1\mathbf{I_{m-1}} \\ & & & & & \mathbf{B} \end{bmatrix},$$

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

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

$\mathbf{P}$ is a matrix of order $(n+1)(m-1)$, and all its block matrices are matrices of order $(m-1)$.

We note that when

$$\mu \leq \frac{c_1}{2\Gamma(2-\alpha)} = \frac{1 - 2^{-\alpha}}{\Gamma(2-\alpha)},$$

we have

$$\begin{aligned} \|P\|_\infty = \max_i \sum_{j=1}^{(n+1)(m-1)} |p_{i,j}| &= \eta + |c_1 - 2\eta| + \eta + c_2 + c_3 + \cdots + c_n + b_n \\ &= c_1 + c_2 + \cdots + c_n + b_n = 1; \end{aligned}$$

where $p_{i,j}$ is the ij^{th} element of the matrix $\mathbf{P}$.

According to the Lax-Richtmer definition of stability [12], we can prove the following theorem:

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

Proof. (See [8])

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,

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

It can be shown that the error vectors satisfy the following matrix form:

$$\begin{cases} \rho_{\mathbf{n+1}} &= \mathbf{Q}\rho_{\mathbf{n}} + \mathbf{S}\ , \quad n \geq 1, \\ \rho_{\mathbf{1}} &= \mathbf{S}. \end{cases} \tag{13}$$

$$\rho_{\mathbf{n+1}} = \begin{bmatrix} \mathbf{E_{n+1}} \\ \vdots \\ \mathbf{E_3} \\ \mathbf{E_2} \end{bmatrix}, \ \mathbf{Q} = \begin{bmatrix} \mathbf{A} & c_2\mathbf{I_{m-1}} & c_3\mathbf{I_{m-1}} & \cdots & c_n\mathbf{I_{m-1}} \\ & & \ddots & \ddots & \vdots \\ & & & \mathbf{A} & c_2\mathbf{I_{m-1}} \\ & & & & \mathbf{A} \end{bmatrix},$$

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

$\mathbf{I_{m-1}}$ is the unit matrix of order $(m-1)$. From which we see that:

$$\begin{aligned} \rho_{\mathbf{n}} &= \mathbf{Q}\rho_{\mathbf{n-1}} + \mathbf{S} \\ &= \left(\mathbf{Q^{n-1}} + \mathbf{Q^{n-2}} + \cdots + \mathbf{Q} + \mathbf{I_{n(m-1)}}\right)\mathbf{S}. \end{aligned} \tag{14}$$

Hence

$$\|\rho_{\mathbf{n}}\|_\infty \leq \tau^\alpha\Gamma(2-\alpha)\cdot O\left(\tau + h^2\right)$$
$$\times\left(\|\mathbf{Q}\|_\infty^{n-1} + \|\mathbf{Q}\|_\infty^{n-2} + \cdots + \|\mathbf{Q}\|_\infty + \|\mathbf{I_{n(m-1)}}\|_\infty\right)$$

We note that $\|\mathbf{I_{n(m-1)}}\|_\infty = 1$ and when $\mu \leq \frac{1-2^{-\alpha}}{\Gamma(2-\alpha)}$, i.e. $c_1 \geq 2\eta$,

$$\|\mathbf{Q}\|_\infty = \eta + |c_1 - 2\eta| + \eta + c_2 + c_3 + \cdots + c_n = \sum_{i=1}^{n} c_i \leq 1$$

Consequently, $\|\rho_\mathbf{n}\|_\infty \leq n\tau^\alpha\Gamma(2-\alpha)\cdot O\left(\tau + h^2\right)$. Note that $n\tau \leq T$ is finite, so that $n\tau^\alpha\Gamma(2-\alpha)$ is also finite. Consequently, when $\tau \to 0$,$h \to 0$ we have $\|\rho_\mathbf{n}\|_\infty \to 0$ and now $\|\mathbf{E_n}\|_\infty \to 0$, thus $|e_{j,n}| \to 0$.

We therefore can write the following result (See [8]):

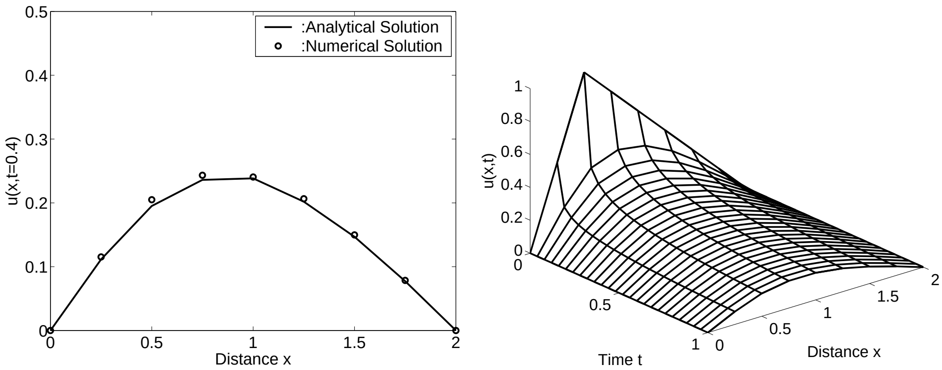
Theorem 2: Let U be the exact solution of the TFDE and y be the approximate solution of the DNMRWA, then y converges to U as h and τ tends to zero when $\mu \leq \frac{1-2^{-\alpha}}{\Gamma(2-\alpha)}$.

Remark 2: We note that the condition for the convergence conforms to the condition for stability, and it is also the scaling restriction (9) for the random walk interpretation.

5 Numerical results

In this section we present an example to demonstrate 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. Here, we take L=2, the evolution results are presented for 1 sec. We take

$$f(x) = \begin{cases} 2x, & 0 \leq x \leq 1/2 \\ (4-2x)/3, & 1/2 \leq x \leq 2. \end{cases}$$

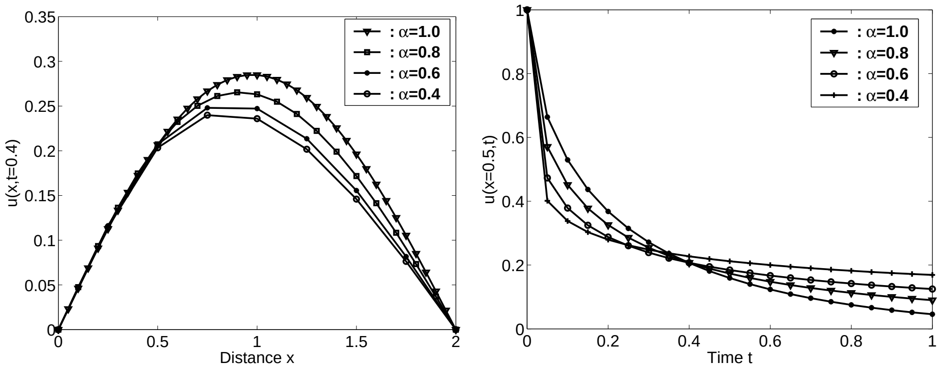


(a) (b)

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 1(a) shows the results of DNMRWA with $h = 0.25$, $\tau = 0.0005$ and the analytical solution for TFDE at $t = 0.4$ and $\alpha = 0.5$. It is apparent from Figure 1 that the numerical solution (DNMRWA) is in good agreement with the analytical solution.

Figure 1(b) shows the evolution result using DNMRWA with $h = 0.25$, $\tau = 0.0005$ for $\alpha = 0.5$. From Figure 2, it can be seen that the $\alpha = 0.5$ order derivative system exhibits fast diffusion in the beginning and slow diffusion later.



(a) (b)

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;

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).

6 Conclusions

The time fractional diffusion equation (TFDE) arrives in a natural way at non-Markovian processes for which space-probability distributions evolve in time consistently with the phenomenon 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 so obtained, with the scaling restriction (9), imitates on a discrete space-time grid the most essential properties of the continuous process, namely conservativity 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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