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Numerical Solution of Diffusion Equation with Caputo Time Fractional Derivatives Using Finite-difference Method with Neumann and Robin Boundary Conditions

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ABSTRACT

Many problems in various branches of science, such as physics, chemistry, and engineering have been recently modeled as fractional ODEs, and fractional PDEs. Thus, methods to solve such equations, especially in the nonlinear state, have drawn the attention of many researchers. The most important goal of researchers in solving such equations has been set to provide a solution with the possible minimum error. The fractional PDEs can be generally classified into two main types, spatial-fractional and time-fractional differential equations. This study was designed to provide a numerical solution for the fractional-time diffusion equation using the finite-difference method with Neumann and Robin boundary conditions. The time fraction derivatives in the concept of Caputo were considered, also the stability and convergence of the proposed numerical scheme has been completely proven and a numerical test was also designed and conducted to assess the efficiency and precision of the proposed method. Eventually it can be said that based on findings, the present technique can provide accurate results.

Keywords: Diffusion equation, Finite-difference, Boundary conditions, Caputo, Stability, and Convergence.

INTRODUCTION:

Fractional diffusion equations have significantly drawn the attention of many scholars due to their use in different branches of science, including their use in describing some phenomena in physics (Metzler and Klafter, 2000), chemistry and biochemistry (Yuste and Lindenberg, 2002), mechanical engineering (Magin *et al.*, 2009), medicine (Chen *et al.*, 2010), and electronics (Kirane *et al.*, 2013). The non-local characteristic appears to be as property and the most important advantage of these equations, indicating that the state of a complex system depends not only on its current state but also on its previous states (Tamsir *et al.*, 2021). Mathematical modeling has been recognized to be one of the strong and fundamental solutions for quantitative and qualitative analysis of such phenomena. In general, the quantitative and qualitative behavior characteristics of complex systems in various science and engineering problems can be much better under-stood by mathematical modeling using fractional differential equations (Tamsir *et al.*, 2021; Demir *et al.*, 2020; Demir and Bayrak, 2019; Demir *et al.*, 2019). Different types of definitions have been suggested for fractional derivatives, including the Riemann-Liouville fractional derivatives and Caputo fractional derivatives as two important applications of them.

Thus, the Caputo fractional derivative is a type of fractional derivative in mathematical modeling with experimental data analysis, which is broadly used in different branches of science. Since the analytical solution of the fractional differential equation, seems to be impossible in many phenomena and their numerical solving would highly matter (Demir *et al.*, 2019; Yavuz *et al.*, 2020; Usta and Sarikaya, 2019).

Considerable numerical methods have been designed for diffusion fractional-time equations. Different authors have employed the finite element (Ford *et al.*, 2011), compact finite element (Jacobs, 2016), Crank-Nicolson (Sayevand *et al.*, 2016), the B-spline-based (Sweilam *et al.*, 2016), and the implicit difference (Zhuang and Liu, 2006) methods to solve fractional-time equations. Murio *et al.* devised a stable unconditional implicit numerical method to solve the one-dimensional linear diffusion fractional-time equation on a finite medium (Murio, 2008). Using the generalized Euler method (GEM), Khader *et al.* proposed numerical methods for solving the fractional Riccati and Logistic differential equations based on Chebyshev approximations (Khader, 2011). Celik *et al.* overcame to examine a numerical method for approximating a fractional diffusion equation, using the Riesz-fractional derivative on finite domains, which has second-order accuracy in terms of time and place. The "fractional central derivative" approach was also used to approximate the Riesz-fractional derivative and the Crank-Nicholson method, which has been applied to the fractional diffusion equation (Çelik and Duman, 2012). In a study, Lin *et al.* analyzed a stable and high-order scheme to effectively solve the fractional-time diffusion equation. Their proposed method relies on finite-difference time scheme and the Legendre spectral methods (Lin and Xu, 2007). A block-oriented finite-difference scheme has been suggested for solution of the fractional-time-diffusion equation on non-uniform networks where unconditional stability and convergence have been proven theoretically (Zhai and Feng, 2016). We considered a Caputo fractional-time diffusion equationin this article using the finite-difference method (FDM). Consider the fractional-time diffusion equation as equation (1) with initial conditions (2) and boundary conditions (3).

$$\frac{\partial^\alpha u(x,t)}{\partial(t)^\alpha} = c(x,t)\frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \qquad 0 < x < L\,, \qquad 0 < t < T, \tag{1}$$

$$u(x,0) = g(x), \qquad 0 < x < L\,, \tag{2}$$

$$u(0,t) = 0,\;\; \omega u(L,t) + \left(c(x,t)\frac{\partial u(x,t)}{\partial x}\right)\Big|_{x=L} = y(t), \qquad 0 < t \le T, \tag{3}$$

In these equations, the condition $0 < \alpha < 1$ is always established, $C\,(x,t)$ is the continuous positive coefficient of the diffusion, $f\,(x,t)$ is the source function, and $g\,(x)$ is a sufficiently smooth function. The presented equations (1) to (3) are assumed to have a unique sufficiently smooth answer for the numerical analysis of the above fractional-time diffusion equation. In equation (3), the boundary conditions have been presented, which is governing this diffusion equation, now we express the Neumann boundary fraction conditions and Robin boundary fraction conditions as $\omega = 0$ and $\omega > 0$, respectively. In these equations, $\frac{\partial^\alpha}{\partial t^\alpha}$ is the Caputo's left fractional derivative (Roul and Goura, 2020; Sayevand *et al.*, 2016; Sun *et al.*, 2013).

$$D_t^\alpha u(x,t) = \frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} + \int_0^t \frac{\partial u(x,s)}{\partial s}\frac{ds}{(t-s)^\alpha}\,, \tag{4}$$

The Taylor expansion has been used in this study to discretize points $u\,(x,t)$ with the third-order accuracy followed by providing a sequence for stability and convergence of the proposed scheme to be proven.

In general, a discretization process has been presented in the section-2 of this literature with an implicit finite-difference, which compatibility has been assessed as well and then in section-3, the stability and convergence of the approach has been proven, as well as a numerical example has been covered in section-4, to know the accuracy and efficiency of the scheme. Finally, the research general conclusion is provided in section-5.

Considering Equations (1) to (3), the temporal and spatial partitions t_m and x_n were defined as equation (5) for their discretization and numerical approximation.

$$x_n = n \times h(n = 0, 1, 2, \dots, N) \& t_m = m \times \tau(m = 0, 1, 2, \dots, M) \tag{5}$$

Where M and N are positive integers and according to the represented partitions, size of the temporal and the spatial networks in the examined discretization would be clearly equal to $\tau = T/M$, and $h = L/N$, respectively. In the process of solving fractional-time diffusion equation in this literature, U_i^m denotes the accurate answer and u_i^m represents the approximate answer resulting from the numerical method at point (x_i, t_m) of the network. Based on assumption, the short equivalent w_i^m is used in this literature for simplifying the writing of equations for all parameters such as $w(x_i, t_m) = w_0$. The lemmas 1 and 2 are used for its discretization by the finite-difference method (Sun & Wu, 2006; Tian *et al.*, 2015).

Providing a model of implicit finite-difference accompanied by evaluating its compatibility

Here, model of implicit finite-difference is presented, accompanied by evaluating its compatibility.

Lemma 1

It was supposed that $0 < \alpha < 1$ and $d(t) \in c^2[0, t_m]$ are established, in such a case, the inequality in (6) would be established as follow.

$$\left| \frac{1}{\Gamma(1-\alpha)} \int_0^{t_m} \frac{d'(s)}{(t_m - s)^\alpha} ds - \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \left(b_0 d(t_m) - \sum_{j=1}^{m-1} (b_{m-j-1} - b_{m-1}) d(t_j) - b_{m-1} d(t_0) \right) \right| \\ \leq \frac{1}{\Gamma(1-\alpha)} \left(\frac{1-\alpha}{12} + \frac{2^{2-\alpha}}{2-\alpha} - (1 + 2^{-\alpha}) \right) \max_{0 \leq t \leq t_m} |d''(t)| \tau^{2-\alpha}, \tag{6}$$

Where, $b_j = (j+1)^{1-\alpha} - j^{1-\alpha}, j = 0, 1, 2, \dots$

Lemma 2

It was supposed that $d(x) \in L^1(R)$ and ${}_{-\infty}D_x^{4} d(x)$ is established and its Fourier transform belongs to $L^1(R)$, and the weighted and transferred Grunwald-Letnikov operator is defined as equation (7) where p and q are integers.

$$L^{D^2_{h,p,q}} d(x) = \frac{\lambda_1}{h^2} \sum_{j=1}^{m-1} g_j^{(2)} d(x - (j-p)h) + \frac{\lambda_2}{h^2} \sum_{j=0}^{\infty} g_j^{(2)} d(x - (j-q)h), \tag{7}$$

In this equation, we knew that $\lambda_1 = \frac{2p-2}{2(p-q)}$ ،$\lambda_2 = \frac{2-2q}{2(p-q)}$ ،$p \neq q$ and $g_j^{(2)} = (-1)^j \binom{2}{j}$ are binominal fractional coefficients. Thus, we would have $L^{D^2_{h,p,q}} d(x) = {}_{-\infty}D_x^{2} d(x) + O(h^2)$. Therefore, we discredited the Caputo fractional-time derivative for each $x \in R$ according to Lemma 1 as equation (8).

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} \Big|_{(x_i, t_{m+1})} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^{m} b_j \left(U_i^{m+1-j} - U_i^{m-j} \right) + O(\tau^{2-\alpha}), \tag{8}$$

Then, according to Lemma 2, the spatial-derivative of equation (1), can be as approximation of equation (9), thus for $p = 1$ and $q = 0$, the spatial-derivative would be discretized as equation (10).

$$\frac{\partial^2 u(x,t)}{\partial x^2} \Big|_{(x_i, t_{m+1})} = \frac{\lambda_1}{h^2} \sum_{j=0}^{i+p} g_j^{(2)} U_{i-j+p}^{m+1} + \frac{\lambda_2}{h^2} \sum_{j=0}^{i+q} g_j^{(2)} U_{i-j+q}^{m+1} + O(h^2). \tag{9}$$

$$\frac{\partial^2 u(x,t)}{\partial x^2} \Big|_{(x_i, t_{m+1})} = \frac{1}{h^2} \sum_{j=0}^{i+1} w_j^{(2)} U_{i-j+1}^{m+1} + O(h^2), \tag{10}$$

Where, $w_0^{(2)} = \frac{2}{2} g_0^{(2)}, w_j^{(2)} = g_j^{(2)}, j = 1,2, \dots, M$ and the first order spatial-derivative on $x = L$ are approximated as equation (11).

$$\frac{\partial u(x,t)}{\partial x}\Big|_{(x_N,t_{m+1})} = \frac{1}{h}\sum_{j=0}^{N+1} w_j\, U_{N-j+1}^{m+1} + O(h^2)\,. \tag{11}$$

Then, we managed to discretize value of U_{N+1}^{m+1} as equation (12) using the third-order Taylor expansion to ultimately decompose equation (11) into equation (13).

$$U_{N+1}^{m+1} = 3U_N^{m+1} - 3U_{N-1}^{m+1} + U_{N-2}^{m+1} + O(h^3)\,. \tag{12}$$

$$\frac{\partial u(x,t)}{\partial x}\Big|_{(x_N,t_{m+1})} = \frac{1}{h}\sum_{j=1}^{N} w_j\, U_{N-j+1}^{m+1} + \frac{w_0}{h}\left(3U_N^{m+1} - 3U_{N-1}^{m+1} + U_{N-2}^{m+1}\right) + O(h^2). \tag{13}$$

It was then supposed that $z = \frac{\tau^\alpha \Gamma(2-\alpha)}{h^2}$ is established, therefore in the case, the implicit finite-difference scheme is written as equations (14) to (17).

$$U_i^1 - zc_i^1 \sum_{j=0}^{N+1} w_j^{(2)}\, U_{i-j+1}^1 = U_i^0 + \tau^\alpha \Gamma(2-\alpha) f_i^1\,, \quad 1 \le i \le N-1 \tag{14}$$

$$U_i^{m+1} - zc_i^{m+1} \sum_{j=0}^{1} w_j^{(2)}\, U_{i-j+1}^{m+1} = (1-b_1)u_i^m + \sum_{j=1}^{m-1}(b_j + b_{j+1})\, u_i^{m-j} + b_m u_i^0 + \tau^\alpha \Gamma(2-\alpha)\, f_i^{m+1},$$
$$1 \le m \le M-1 \quad \& 1 \le i \le N-1 \tag{15}$$

$$U_0^{m+1} = 0, \qquad 0 \le m \le M-1 \quad \& \mathrm{i} = \mathrm{N} \tag{16}$$

$$\omega u_N^{m+1} + \frac{c_N^{m+1}}{h}\sum_{j=1}^{N} w_j\, U_{N-j+1}^{m+1} + \frac{c_N^{m+1} w_0}{h}\left(3U_N^{m+1} - 3U_{N-1}^{m+1} + U_{N-2}^{m+1}\right) = y^{m+1},$$
$$0 \le m \le M-1 \quad \& \mathrm{i} = \mathrm{N} \tag{17}$$

After analyzing local truncation-error for $1 \le i \le N$ with R_i^m, the value of error can be seen with using equations (8), (10), and (13) as follows. In fact, this issue implies that, compatibility of implicit finite-difference schemes defined by (14) to (17) is:

$$R_i^1 = U_i^1 - zc_i^1 \sum_{j=0}^{i} w_j^{(2)}\, U_{i-j+1}^1 - U_i^0 - \tau^\alpha \Gamma(2-\alpha) f_i^1 = O(\tau^{2-\alpha} + h^2), 1 \le i \le N-1, \tag{18}$$

$$R_i^{m+1} = U_i^{m+1} - zc_i^{m+1} \sum_{j=0}^{i} w_j^{(2)}\, U_{i-j+1}^{m+1} - (1-b_1)U_i^m - \sum_{j=1}^{m-1}\left(b_j - b_{j+1}\right) U_i^{m-j} - b_m U_i^0$$
$$- \tau^\alpha \Gamma(2-\alpha) f_i^{m+1} = O(\tau^{2-\alpha} + h^2), \quad 1 \le i \le N-1, \quad 1 \le m \le M-1, \tag{19}$$

$$R_N^{m+1} = \omega U_N^{m+1} + \frac{c_N^{m+1}}{h}\sum_{j=1}^{N} w_j\, U_{N-j+1}^{m+1} + \frac{c_N^{m+1} w_0}{h}\left(3U_N^{m+1} - 3U_{N-1}^{m+1} + U_{N-2}^{m+1}\right) - y^{m+1} = O(h^2),$$
$$0 \le m \le M-1. \tag{20}$$

the form of a matrix shown in (21) for elucidation of the text. By using provided matrix definition, we expressed the implicit finite-difference scheme discretized in Equations (14) to (17) as a matrix shown in Equations (22) and (23).

The stability analysis and convergence

In this section of literature, stability and convergence of finite numerical difference has been discussed for solving the fractional-time diffusion equation. The columnar vectors U^m, Q^{m-1}, and F^m are defined in

$$\begin{cases} U^m = (u_1^m, u_2^m, \dots, u_N^m)^T, \\ V^{m-1} = (u_1^{m-1}, u_2^{m-1}, \dots, u_{N-1}^{m-1}, 0)^T, \\ W^m = (\tau^\alpha \Gamma(2-\alpha) f_1^m, \tau^\alpha \Gamma(2-\alpha) f_2^m, \dots, \tau^\alpha \Gamma(2-\alpha) f_{N-1}^m, hy^m)^T, \end{cases} \quad for\ 1 \le m \le M \tag{21}$$

$$AU^1 = V^0 + W^1, \quad 1 \le m \le M-1 \tag{22}$$

$$AU^{m+1} = (1-b_1)V^m + \sum_{j=1}^{m-1}(b_j - b_{j+1})V^{m-j} + b_m V^0 + W^{m+1}, \qquad 1 \le m \le M-1 \tag{23}$$

The coefficients of elements in above matrix can be as form of matrix A, which is elucidated in equation (24).

$$A = \begin{cases} zc_i^{m+1} w_{i-j+1}^{(2)}, & 1 \le j \le i-1, \quad 1 \le i \le N-1, \\ 1 - zc_i^{m+1} w_1^{(2)}, & 1 \le j = i \le N-1, \\ -zc_i^{m+1} w_0^{(2)}, & j = i+1, \quad 1 \le i \le N-1, \\ 0, & i+2 \le j \le N, \quad 1 \le i \le N-2, \\ c_N^{m+1} w_{N-j+1}, & 1 \le j \le N-3, \quad i = N, \\ c_N^{m+1} w_3 + c_N^{m+1} w_0, & j = N-2, \quad i = N, \\ c_N^{m+1} w_2 - 3c_N^{m+1} w_0, & j = N-1, \quad i = N, \\ h\omega + c_N^{m+1} w_1 + 3c_N^{m+1} w_0, & j = i = N. \end{cases} \tag{24}$$

Some lemmas, as bellow are needed to evaluate the sustainability of the mentioned scheme (Samko *et al.*, 1993; Liu *et al.*, 2015; Lin and Xu, 2007).

Lemma 3

It was supposed that ρ includes positive real numbers and$n \ge 1$ is an integer. In such a case, the coefficients $f_j^{(\rho)} (j = 0,1,..)$ would have properties as following:

$$f_0^{(\rho)} = 1, \qquad f_j^{(\rho)} = \left(1 - \frac{\rho+1}{j}\right) f_{j-1}^{(\rho)} \qquad for\ j \ge 1, \tag{i}$$

$$f_1^{(\rho)} < f_2^{(\rho)} < \cdots < 0, \sum_{j=0}^{n} f_j^{(\rho)} > 0 \qquad for\ 0 < \rho < 1, (ii)$$

$$f_2^{(\rho)} > f_3^{(\rho)} > \cdots > 0, \sum_{j=0}^{n} f_j^{(\rho)} > 0 \qquad for\ 1 < \rho < 2, \tag{iii}$$

$$\sum_{j=0}^{n} f_j^{(\rho)} = (-1)^n \binom{\rho-1}{n}, \tag{iv}$$

$$\sum_{j=0}^{n} f_j^{(\rho_1)} = f_{n-j}^{(\rho_2)} = f_n^{(\rho_1+\rho_2)}. \tag{v}$$

Lemma 4

It was supposed that ρ is positive real value, where the case, $w_j^{(\rho)} (j = 0,1,\dots)$ would have some of the properties, as expressed bellow.

$$w_0^{(\rho)} = \frac{\rho}{2}, w_0^{(\rho)} = \frac{2-\rho-\rho^2}{2}, w_2^{(\rho)} = \frac{\rho(\rho^2+\rho-4)}{2}, \tag{i}$$

$$w_0^{(\rho)} = \frac{\rho}{2} f_j^{(\rho)} + \frac{2-\rho}{2} f_{j-1}^{(\rho)}, \qquad for\ j \ge 3, \tag{ii}$$

$$w_2^{(\rho)} \leq w_3^{(\rho)} \leq \cdots \leq 0, \qquad \sum_{j=0}^{n} w_j^{(\rho)} > 0, \quad for\ 0 < \rho < 1, \qquad n \geq 1, \qquad (iii)$$

$$1 > w_0^{(\rho)} > w_3^{(\rho)} > w_4^{(\rho)} \ldots > 0, \sum_{j=0}^{n} w_j^{(\rho)} < 0, \quad for\ 1 < \rho < 2, \qquad n \geq 2. \qquad (iv)$$

Lemma 5

If ρ_1 and ρ_2 are supposed as two constants, in such case, the coefficients $b_j (j = 1,2, \ldots)$ would be dealt with properties, written below.

$$b_{j>0}, \qquad (i)$$

$$b_j > b_{j+1}, \qquad (ii)$$

$$\rho_1 j^{\alpha} \leq (b_j)^{-1} \leq \rho_2 j^{\alpha}. \qquad (iii)$$

We considered the error value $\varepsilon_i^m = u_i^m - \tilde{u}_i^m$, where stability of the numerical method of implicit finite-difference provided scheme for solving the fractional-time diffusion equation is evaluated. Hence, $\tilde{u}_i^m$ is obtained as the approximate answer of the differential scheme with the initial condition $\tilde{u}_i^0$. In such a situation, the error value of the matrix form will be as defined in equation (25).

$$\varepsilon^m = (\varepsilon_1^m, \varepsilon_1^m, \ldots, \varepsilon_N^m)^T, \qquad \|\varepsilon^m\|_\infty = \max_{1 \leq i \leq N} |\varepsilon_i^m|. \qquad (25)$$

Then, according to the definition of the finite-difference scheme provided in this literature, we obtain:

$$\varepsilon_i^1 - zc_i^1 \sum_{j=0}^{i} w_j^{(2)} \varepsilon_{i-j+1}^{m+1} = \varepsilon_i^0, \qquad 1 \leq i \leq N-1, 1 \leq m \leq M-1, \qquad (26)$$

$$\varepsilon_i^{m+1} - zc_i^{m+1} \sum_{j=0}^{i} w_j^{(2)} \varepsilon_{i-j+1}^{m+1} = (1-b_1)\varepsilon_i^m + \sum_{j=1}^{m-1} (b_j - b_{j+1}) \varepsilon_i^{m-j} + b_m \varepsilon_i^0,$$
$$1 \leq i \leq N-1 \quad, 1 \leq m \leq M-1, \qquad (27)$$

$$\omega \varepsilon_N^{m+1} + \frac{c_N^{m+1}}{h} \sum_{j=1}^{N} w_j \varepsilon_{N-j+1}^{m+1} + \frac{c_N^{m+1} w_0}{h} (3\varepsilon_N^{m+1} - |3\varepsilon_{N-1}^{m+1} + \varepsilon_{N-2}^{m+1}) = 0, \qquad i = N, \varepsilon_0^m (m = 0,1, \ldots, M),$$
$$0 \leq m \leq M-1. \qquad (28)$$

Then, using equation (28), we obtained equation (29). Afterward, considering the $i = N-1$, we achieved equations (30) and (31) by substituting equation (29) in equations (26) and (27).

$$\varepsilon_N^{m+1} = \frac{-c_N^{m+1} \sum_{j=2}^{N} w_j \varepsilon_{N-j+1}^{m+1} + 3c_N^{m+1} w_0 \varepsilon_{N-1}^{m+1} - c_N^{m+1} w_0 \varepsilon_{N-2}^{m+1}}{h\omega + c_N^{m+1} w_1 + 3c_N^{m+1} w_0}, \qquad (29)$$

$$\varepsilon_{N-1}^1 - zc_{N-1}^1 \sum_{j=1}^{N-1} (w_{N-1}^{(2)} - s^1 c_N^1 w_0^{(2)} w_{N-j+1}) \varepsilon_j^1 - 3zs^1 c_{N-1}^1 c_N^1 w_0^{(2)} w_0 \varepsilon_{N-1}^1 + zs^1 c_{N-1}^1 c_N^1 w_0^{(2)} w_0 \varepsilon_{N-2}^1$$
$$= \varepsilon_{N-1}^0, \qquad (30)$$

$$\varepsilon_{N-1}^{m+1} - zc_{N-1}^{m+1} \sum_{j=1}^{N} (w_{N-1}^{(2)} - s^{m+1} c_N^{m+1} w_0^{(2)} w_{N-j+1}) \varepsilon_j^{m+1} - 3zs^{m+1} c_{N-1}^{m+1} c_N^{m+1} w_0^{(2)} w_0 \varepsilon_{N-1}^{m+1}$$
$$+ zs^{m+1} c_{N-1}^{m+1} c_N^{m+1} w_0^{(2)} w_0 \varepsilon_{N-2}^{m+1}$$
$$= (1-b_1)\varepsilon_{N-1}^m + \sum_{j=1}^{m-1} (b_j - b_{j+1}) \varepsilon_{N-1}^{m-j} + b_m \varepsilon_{N-1}^0, \qquad (31)$$

Proof

We first defined matrix of the function ξ in the form of $\xi^m = (\varepsilon_1^m, \varepsilon_2^m, \ldots, \varepsilon_{N-1}^m)^T, 1 \le m \le M$. In such a case, equations $(26), (27), (30)$ and (31) can be obtained as follows.

Following the discussion and we prove theorem-1 for stability of the mentioned numerical method as following.

Theorem 1

The implicit finite-difference presented for the fractional-time diffusion equation (14) - (17) is unconditionally stable.

$$B\xi^1 = \xi^0, \qquad 1 \le m \le M-1, \tag{32}$$

$$B\xi^{m+1} = (1-b_1)\xi^m + \sum_{j=1}^{m-1}(b_j - b_{j+1})\xi^{m-j} + b_m\xi^0, \qquad 1 \le m \le M-1, \tag{33}$$

Then, the coefficients of elements in matrix B will be calculated as shown in equation (34).

$$B = \begin{cases} -zc_i^{m+1}w_{i-j+1}^{(2)}, & 1 \le j \le i-1, \quad 1 \le i \le N-1, \\ 1 - zc_i^{m+1}w_1^{(2)}, & 1 \le j = i \le N-2, \\ -zc_i^{m+1}w_0^{(2)}, & j = i+1, \quad 1 \le i \le N-1, \\ 0, & i+2 \le j \le N-1, \quad 1 \le i \le N-3, \\ -zc_{N-1}^{m+1}(w_{N-j}^{(2)} - s^{m+1}c_N^{m+1}w_0^{(2)}w_{N-j+1}), & 1 \le j \le N-3, \quad i = N-1, \\ -zc_{N-1}^{m+1}(w_2^{(2)} - s^{m+1}c_N^{m+1}w_0^{(2)}w_3 - s^{m+1}c_N^{m+1}w_0^{(2)}w_0), j = N-2, i = N-1, \\ 1 - zc_{N-1}^{m+1}(w_1^{(2)} - s^{m+1}c_N^{m+1}w_0^{(2)}w_2 + 3s^{m+1}c_N^{m+1}w_0^{(2)}w_0), i = j = N-1. \end{cases} \tag{34}$$

For proof of the theorem, firstly it is needed to show that matrix B, does not have unique eigenvalue. To prove this issue, we indicated that eigenvalues of matrix B fall within circles, having center $b_{i,j}$ and radius $\sum_{j=1,j\ne i}^{N-1}|b_{i,j}|$, according to Gerschgorin theorem (Xie and Fang, 2019). Thus, based on Lemma 4:

$$b_{i,j} \le 0, \quad j \ne i, \qquad 1 \le i \le N-1, \tag{35}$$

$$b_{i,j} \ge 1, 1 \le i \le N-1, \tag{36}$$

The result will be as:

$$b_{i,j} - \sum_{j=1,j\ne i}^{N-1}|b_{i,j}| = \sum_{j=1}^{N-1} b_{i,j} = 1 - zc_i^{m+1}\sum_{j=0}^{i} w_j^{(2)} > 1. \tag{37}$$

On the other hand, according to Lemma 3 and Lemma 4, it can be written that:

$$s^{m+1}c_N^{m+1} = \frac{c_N^{m+1}}{h\omega + c_N^{m+1}w_1 + 3c_N^{m+1}w_0} \le \frac{c_N^{m+1}}{c_N^{m+1}w_1 + 3c_N^{m+1}w_0} = \frac{1}{w_1 + 3w_0} < 1. \tag{38}$$

Then, direct calculation led to:

$$w_3 + w_0 > 0, \qquad -w_2^{(2)} + w_0^{(2)}w_3 + w_0^{(2)}w_0 < 0, \qquad -w_1^{(2)} + w_0^{(2)}w_2 + 3w_0^{(2)}w_0 > 0. \tag{39}$$

Therefore, we reached the following equations:

$$b_{N-1,j} = zc_{N-1}^{m+1}\left(w_{N-j}^{(2)} - s^{m+1}c_N^{m+1}w_0^{(2)}w_{N-j+1}\right) \le 0, \qquad 1 \le j \le N-3, \mathrm{i} = \mathrm{N}-1, \tag{40}$$

$$b_{N-1,N-2} = zc_{N-1}^{m+1}\left(-w_2^{(2)} + s^{m+1}c_N^{m+1}w_0^{(2)}(w_3 + w_0)\right) < zc_{N-1}^{m+1}\left(-w_2^{(2)} + w_0^{(2)}(w_3 + w_0)\right) < 0,$$
$$\mathrm{i} = \mathrm{N} - 1. \tag{41}$$

$$b_{N-1,N-2} = 1 + zc_{N-1}^{m+1}\left(-w_1^{(2)} + s^{m+1}c_N^{m+1}w_0^{(2)}w_2 - 3s^{m+1}c_N^{m+1}w_0^{(2)}w_0\right)$$
$$> 1 + zc_{N-1}^{m+1}\left(-w_1^{(2)} + w_0^{(2)}w_2 - 3w_0^{(2)}w_0\right) > 1, \qquad \mathrm{i} = \mathrm{N} - 1. \tag{42}$$

The above three equations came to the conclusion below:

$$b_{N-1,N-1}-\sum_{j=1}^{N-2}\left|b_{i,j}\right|=\sum_{j=1}^{N-1}b_{i,j}=1+zc_{N-1}^{m+1}\left(-\sum_{j=1}^{N-1}w_j^{(2)}+s^{m+1}c_N^{m+1}w_0^{(2)}\sum_{j=2}^{N}w_j-2s^{m+1}c_N^{m+1}w_0^{(2)}w_0\right)$$
$$>1+zc_{N-1}^{m+1}\left(w_0^{(2)}-s^{m+1}c_N^{m+1}w_0^{(2)}w_0+w_1)-2s^{m+1}c_N^{m+1}w_0^{(2)}w_0\right)$$
$$>1+zc_{N-1}^{m+1}\left(w_0^{(2)}-\frac{w_0^{(2)}(c_N^{m+1}w_1+3c_N^{m+1}w_0)}{h\omega+c_N^{m+1}w_1+3c_N^{m+1}w_0}\right)>1. \tag{43}$$

The inequalities shown in equations (37) and (43) suggests that matrix B, does not have unique eigenvalue. Thus, spectral radius of matrix B^{-1}, was found to be less than one, so by following the process, it is advised to show that equation (44) is established.

$$\left\|\xi^{m}\right\|_{\infty}\le\left\|\xi^{0}\right\|_{\infty},\qquad 1\le m\le M. \tag{44}$$

In fact, according to (32), we are writing:

$$\left\|\xi^{1}\right\|_{\infty}\le\left\|\xi^{0}\right\|_{\infty}, \tag{45}$$

Assuming the establishment of equation (46) and according to equation(33), equation(47), it is obtained as:

$$\left\|\xi^{k}\right\|_{\infty}\le\left\|\xi^{0}\right\|_{\infty},\quad k=2,3,\dots,m. \tag{46}$$

$$\left\|\xi^{k+1}\right\|_{\infty}\le\left\|(1-b_1)\xi^{k}+\sum_{j=1}^{k-1}(b_j-b_{j+1})\,\xi^{k-1}+b_k\xi^{0}\right\|_{\infty}\le_{\infty}(1-b_1)\left\|\xi_1^{k}\right\|_{\infty}$$
$$+\sum_{j=1}^{k-1}(b_j-b_{j+1})\left\|\xi_1^{k-j}\right\|_{\infty}+b_k\left\|\xi_1^{0}\right\|_{\infty}\le\left((1-b_1)+\sum_{j=1}^{k-1}(b_j-b_{j+1})+b_k\right)\left\|\xi^{0}\right\|_{\infty}$$
$$=\left\|\xi^{0}\right\|_{\infty}. \tag{47}$$

By using mathematical induction, it is managed to obtain equation (44) and on the other hand, value of $\left|\varepsilon_N^{m+1}\right|$ is calculated as:

$$\left|\varepsilon_N^{m+1}\right|=\frac{\left|c_N^{m+1}\sum_{j=2}^{N}w_j\varepsilon_{N-j+1}^{m+1}-3c_N^{m+1}w_0\varepsilon_{N-1}^{m+1}+c_N^{m+1}w_0\varepsilon_{N-2}^{m+1}\right|}{\left|h\omega+c_N^{m+1}w_1+3c_N^{m+1}w_0\right|},$$
$$\le\frac{\left|c_N^{m+1}\sum_{j=2}^{N}\left|w_j\right|\left|\varepsilon_{N-j+1}^{m+1}\right|+3c_N^{m+1}w_0\left|\varepsilon_{N-1}^{m+1}\right|+c_N^{m+1}w_0\left|\varepsilon_{N-2}^{m+1}\right|\right|}{h\omega+c_N^{m+1}w_1+3c_N^{m+1}w_0},$$
$$\le\frac{c_N^{m+1}\left(\sum_{j=2}^{N}\left|w_j\right|+4w_0\right)}{h\omega+c_N^{m+1}w_1+3c_N^{m+1}w_0}\max_{1\le i\le N-1}\left|\varepsilon_i^{m+1}\right|\le\frac{c_N^{m+1}(w_1+5w_0)}{h\omega+c_N^{m+1}w_1+3c_N^{m+1}w_0}\max_{1\le i\le N-1}\left|\varepsilon_i^{m+1}\right|,$$
$$\le\frac{\frac{5}{3}c_N^{m+1}(w_1+3w_0)}{h\omega+c_N^{m+1}w_1+3c_N^{m+1}w_0}\max_{1\le i\le N-1}\left|\varepsilon_i^{m+1}\right|\le\frac{5}{3}\max_{1\le i\le N-1}\left|\varepsilon_i^{m+1}\right|\le\frac{5}{3}\left\|\xi^{m+1}\right\|_{\infty}\le\frac{5}{3}\left\|\xi^{0}\right\|_{\infty},$$
$$i=N. \tag{48}$$

Using equations (44) and (48), then it is obtained that:

$$\|\varepsilon^{m+1}\|_{\infty}=\max\left\{\left\|\xi^{m+1}\right\|_{\infty},\left|\varepsilon_N^{m+1}\right|\right\}\le C\left\|\xi^{0}\right\|_{\infty}\le C\|\varepsilon^{0}\|_{\infty}. \tag{49}$$

Here C is positive constant coefficient and it is independent of τ and h. Hence, the argument was completed according to (Smith *et al.*, 1985; Yu and Tan, 2003). Afterward, we defined e_i^m and its matrix as form of equations (50) and (51), to continue the assessment of numerical convergence of the method presented in this literature.

$$e_i^m = U_i^m - u_i^m, \qquad 1 \le i \le N, 0 \le m \le M, \tag{50}$$

$$e^m = (e_1^m, e_2^m, \dots, e_N^m)^T, \qquad \|e^m\|_\infty = \max_{1\le i\le N} |e_i^m|. \tag{51}$$

Alternatively, according to the definition of finite-difference scheme for $1 \le i \le N-1$ and $1 \le m \le M-1$, we achieved following equations:

$$e_i^1 - zc_i^1 \sum_{j=0}^{i} w_j^{(2)} e_{i-j+1}^1 = e_i^0 + \tau^\alpha \Gamma(2-\alpha) R_i^1, \tag{52}$$

$$\begin{aligned} e_i^{m+1} - zc_i^{m+1} \sum_{j=0}^{i} w_j^{(2)} e_{i-j+1}^{m+1} \\ &= (1-b_1)e_i^m + \sum_{j=1}^{m-1} (b_j - b_{j+1}) e_i^{m-j} + b_m e_i^0 \\ &+ \tau^\alpha \Gamma(2-\alpha) R_i^{m+1}, \end{aligned} \tag{53}$$

Where, $i = N$ and $0 \le m \le M-1$, $\varepsilon_0^m (m = 0,1,\dots,M)$:

$$\omega e_N^{m+1} + \frac{c_N^{m+1}}{h} \sum_{j=1}^{N} w_j e_{N-j+1}^{m+1} + \frac{c_N^{m+1} w_0}{h} (3e_N^{m+1} - 3e_{N-1}^{m+1} + e_{N-2}^{m+1}) = R_N^{m+1}, \tag{54}$$

Based on (54), the equation below was obtained:

$$e_N^{m+1} = \frac{-c_N^{m+1} \sum_{j=2}^{N} w_j e_{N-j+1}^{m+1} + 3c_N^{m+1} w_0 e_{N-1}^{m+1} - c_N^{m+1} w_0 e_{N-2}^{m+1} + hR_N^{m+1}}{h\omega + c_N^{m+1} w_1 + 3c_N^{m+1} w_0}, \tag{55}$$

Supposing, that $i = N-1$ is established and equations (56) and (57) are obtained by placing (55) in relations (52) and (53).

$$\begin{aligned} e_{N-1}^1 - zc_{N-1}^1 \sum_{j=1}^{N-1} (w_{N-j}^{(2)} - s^1 c_N^1 w_0^{(2)} w_{N-j+1}) e_j^1 - 3zs^1 c_{N-1}^1 c_N^1 w_0^2 w_0 e_{N-1}^1 + zs^1 c_{N-1}^1 c_N^1 w_0^{(2)} w_0 e_{N-2}^1 \\ = e_{N-1}^0 + \tau^\alpha \Gamma(2-\alpha) \bar{R}_{N-1}^{m+1}, \end{aligned} \tag{56}$$

$$\begin{aligned} e_{N-1}^{m+1} - zc_{N-1}^{m+1} \sum_{j=1}^{N-1} (w_{N-j}^{(2)} - s^{m+1} c_N^{m+1} w_0^{(2)} w_{N-j+1}) e_j^{m+1} - 3zs^{m+1} c_{N-1}^{m+1} c_N^{m+1} w_0^{(2)} w_0 e_{N-1}^{m+1} \\ + zs^{m+1} c_{N-1}^{m+1} c_N^{m+1} w_0^{(2)} w_0 e_{N-2}^{m+1} \\ = (1-b_1) e_{N-1}^m + \sum_{j=1}^{m-1} (b_j - b_{j+1}) e_{N-1}^{m-j} + b_m e_{N-1}^0 + \tau^\alpha \Gamma(2-\alpha) \bar{R}_{N-1}^{m+1}, \end{aligned} \tag{57}$$

Where, $\bar{R}_{N-1}^{m+1} \le C(\tau^{2-\alpha} + h^2)$ is established. Now here we present and prove Theorem-2 for convergence of the method.

Theorem 2

The implicit finite-difference scheme expressed in equations (14) to (17) is an unconditional convergence and the constant α constant is independent of τ and h so that –

$$\|U_i^m - u_i^m\|_\infty \le C(\tau^{2-\alpha} + h^2), \quad 1 \le m \le M \tag{58}$$

Proof

We first put $\zeta^m = (e_1^m, e_2^m, \dots, e_{N-1}^m)^T, 1 \le m \le M$. Therefore, we could write equations (52), (53), (56), and (57) as follow:

$$B\zeta^{m+1} = \zeta^0 + R^1, \tag{59}$$

$$B\zeta^{m+1} = (1-b_1)\zeta^m + \sum_{j=1}^{m-1}(b_j - b_{j+1})\zeta^{m-j} + b_m\zeta^0 + R^m, \tag{60}$$

Where, $R^m = \tau^\alpha \Gamma(2-\alpha)(R_1^m, R_2^m, \dots, R_{N-2}^m, R_{N-1}^{-m+1})^T$. In case of $m = 0$, it is followed as below:

$$\max_{1\le i\le N-1}|e_i^1| = \|\zeta^1\|_\infty \le \|\zeta^0\|_\infty + \|R^1\|_\infty \le C\tau^\alpha(\tau^{2-\alpha}+h^2) = b_0^{-1}C\tau^\alpha(\tau^{2-\alpha}+h^2), \tag{61}$$

Where, C is positive constant, which is independent of τ and h. Now it is supposed that:

$$\max_{1\le i\le N-1}|e_i^k| = \|\zeta^k\|_\infty \le b_{k-1}^{-1}C\tau^\alpha(\tau^{2-\alpha}+h^2), \tag{62}$$

Where, $k = 2, 3, \dots, m$ and $C$is constant independent of τ and h, due to $b_m \le b_k \le 1$:

$$b_m^{-1} \ge b_k^{-1}. \tag{63}$$

Therefore, equation (62) can be expressed as form of equation (64).

$$\max_{1\le i\le N-1}|e_i^k| = \|\zeta^k\|_\infty \le b_m^{-1}C\tau^\alpha(\tau^{2-\alpha}+h^2). \tag{64}$$

Therefore:

$$\begin{aligned}\max_{1\le i\le N-1}|e_i^{k+1}| = \|\zeta^{k+1}\|_\infty &\le \left\|(1-b_1)\zeta^k + \sum_{j=1}^{k-1}(b_j-b_{j+1})\zeta^{k-j} + b_k\zeta^0 + R^{k+1}\right\|_\infty, \\ &\le (1-b_1)\|\zeta^k\|_\infty + \sum_{j=1}^{k-1}(b_j-b_{j+1})\|\zeta^{k-1}\|_\infty + \|R^{k+1}\|_\infty, \\ &\le \left((1-b_1) + \sum_{j=1}^{k-1}(b_j-b_{j+1}) + b_m\right)b_m^{-1}C\tau^\alpha(\tau^{2-\alpha}+h^2), \\ &< b_m^{-1}C\tau^\alpha(\tau^{2-\alpha}+h^2).\end{aligned} \tag{65}$$

The equation below can be obtained by the method of mathematical induction:

$$\begin{aligned}\max_{1\le i\le N-1}|e_i^{m+1}| = \|\zeta^{m+1}\|_\infty \le b_m^{-1}C\tau^\alpha(\tau^{2-\alpha}+h^2) \le C_1(m\tau)^\alpha(\tau^{2-\alpha}+h^2) \\ \le C_2(\tau^{2-\alpha}+h^2),\end{aligned} \tag{66}$$

Where, $0 \le m \le M-1$, and C_1 and C_2 are positive constants independent of τ and h. also for $i = N$, we would have:

$$\begin{aligned}|e_N^{m+1}| &= \frac{\left|-c_N^{m+1}\sum_{j=2}^N w_j e_{N-j+1}^{m+1} + 3c_N^{m+1}w_0 e_{N-1}^{m+1} - c_N^{m+1}w_0 e_{N-2}^{m+1} + hR_N^{m+1}\right|}{\left|h\omega + c_N^{m+1}w_1 + 3c_N^{m+1}w_0\right|}, \\ &\le \frac{c_N^{m+1}\sum_{j=2}^N|w_j||e_{N-j+1}^{m+1}| + 3c_N^{m+1}w_0 e_{N-1}^{m+1} + c_N^{m+1}w_0|e_{N-2}^{m+1}| + h|R_N^{m+1}|}{h\omega + c_N^{m+1}w_1 + 3c_N^{m+1}w_0}, \\ &\le \frac{c_N^{m+1}(\sum_{j=2}^N|w_j| + 4w_0)}{h\omega + c_N^{m+1}w_1 + 3c_N^{m+1}w_0}\max_{1\le i\le N-1}|e_i^{m+1}| + \frac{h|R_N^{m+1}|}{c_N^{m+1}w_1 + 3c_N^{m+1}w_0}, \\ &\le \frac{c_N^{m+1}(w_1 + 5w_0)}{h\omega + c_N^{m+1}w_1 + 3c_N^{m+1}w_0}\max_{1\le i\le N-1}|e_i^{m+1}| + \frac{h|R_N^{m+1}|}{c_N^{m+1}w_1 + 3c_N^{m+1}w_0}, \\ &\le \frac{\frac{5}{3}c_N^{m+1}(w_1 + 3w_0)}{h\omega + c_N^{m+1}w_1 + 3c_N^{m+1}w_0}\max_{1\le i\le N-1}|e_i^{m+1}| + \frac{h|R_N^{m+1}|}{c_N^{m+1}w_1 + 3c_N^{m+1}w_0}, \\ &\le \frac{5}{3}\max_{1\le i\le N-1}|e_i^{m+1}| + \frac{h|R_N^{m+1}|}{c_N^{m+1}w_1 + 3c_N^{m+1}w_0} \\ &\le \frac{5}{3}\left\|\xi^{m+1}\right\|_\infty + \frac{h|R_N^{m+1}|}{c_N^{m+1}w_1 + 3c_N^{m+1}w_0} \le C_3\,(\tau^{2-\alpha} \\ &+ h^2).\end{aligned} \tag{67}$$

Where, $0 \leq m \leq M-1$ and C_3 is a positive coefficient, which is independent of τ and h. Based on (66) and (67), it was followed as below:

$$\|e^{m+1}\|_\infty = max\{\|\zeta^{m+1}\|_\infty, |e_N^{m+1}|\} \leq C\,(\tau^{2-\alpha} + h^2). \tag{68}$$

Where, C is positive constant and it is independent of τ and h. Thereby, the argument was completed.

Numerical examples

The efficiency and consistency of numerical method, presented for the Caputo fractional-time diffusion equation is determined in this section, which is followed by considering the maximum error indices L_2 and L_{max} for this evaluation.

$$L_2 = \sqrt{h \sum_{j=0}^{M} \left|u_j^{exact} - u_j^{numerical}\right|^2}\,, \qquad L_{max} = \max_{0\leq j\leq M} \left|u_j^{exact} - u_j^{numerical}\right|, \tag{69}$$

The ROC of this problem is calculated as follow:

$$ROC = \frac{log(E^{h_1}/E^{h_2})}{log(h_1/h_2)}, \qquad ROC = \frac{log(E^{k_1}/E^{k_2})}{log(k_1/k_2)}\,, \tag{70}$$

Where, the errors E^{h_1} and E^{h_2} of size h_1 and h_2 are presented here respectively and as well as E^{k_1} and E^{k_2} indicate, errors in the mesh sizes k_1 and k_2 respectively.

Example

We initially considered the Caputo fractional-time diffusion equation:

$$\frac{\partial^\alpha u(x,t)}{\partial (t)^\alpha} = c(x,t)\frac{\partial^2 u(x,t)}{\partial x^2} + f(x,t), \qquad 0 < x < L\,, \qquad 0 < t < T, \qquad 0 < \alpha < 1.$$

Considering the:

$$f(x,t) = \left(\frac{2}{\Gamma(3-\alpha)} t^{2-\alpha} + 4\pi^2 t^2\right), \quad c(x,t) = 1, \quad y(x,t) = 2\pi t^2, \quad u(0,t) = 0, \quad u(x,0) = 0.$$

The accurate answer will be equal to $u(x,t) = t^2 \sin(2\pi x)$.

Result of the numerical and analytical solutions of this problem is illustrated in Figures 1-3 by using the method provided in this literature.

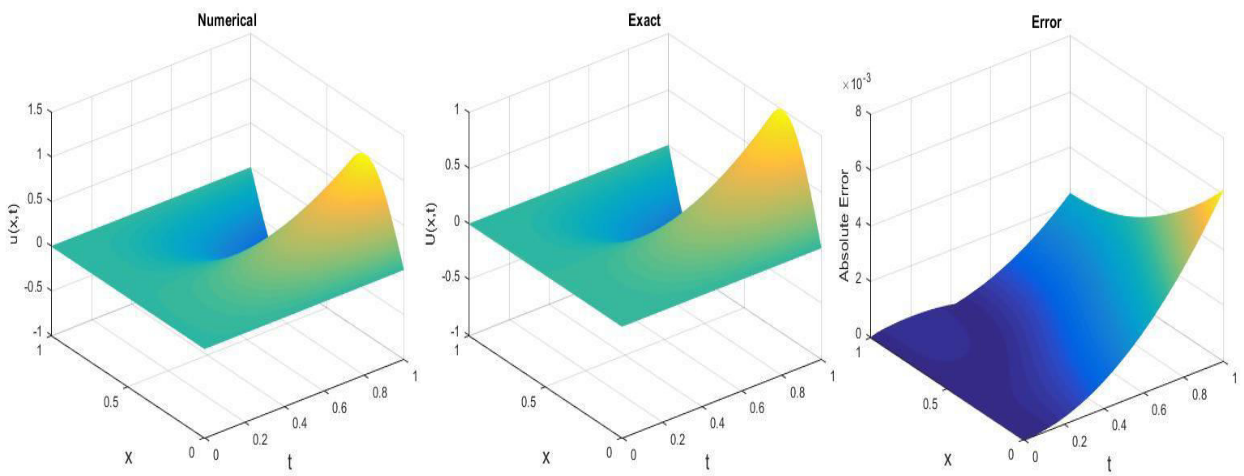

Fig. 1: Shows result of analytical and approximate solutions and as well as absolute error with $\Delta x = 2^{-10}$ and $\Delta t = 2^{-7}$.

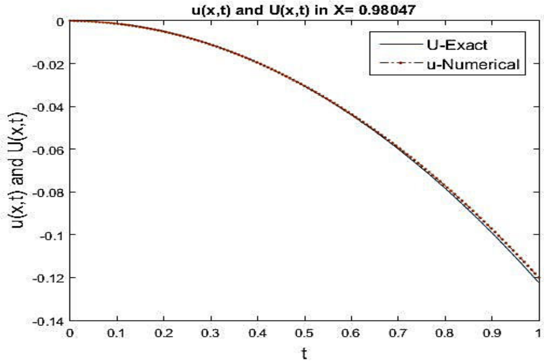

Fig. 2: Shows results of analytical and approximate solution at $x \approx 1$ for $\Delta x = 2^{-10}$ and $\Delta t = 2^{-7}$at different t_S.

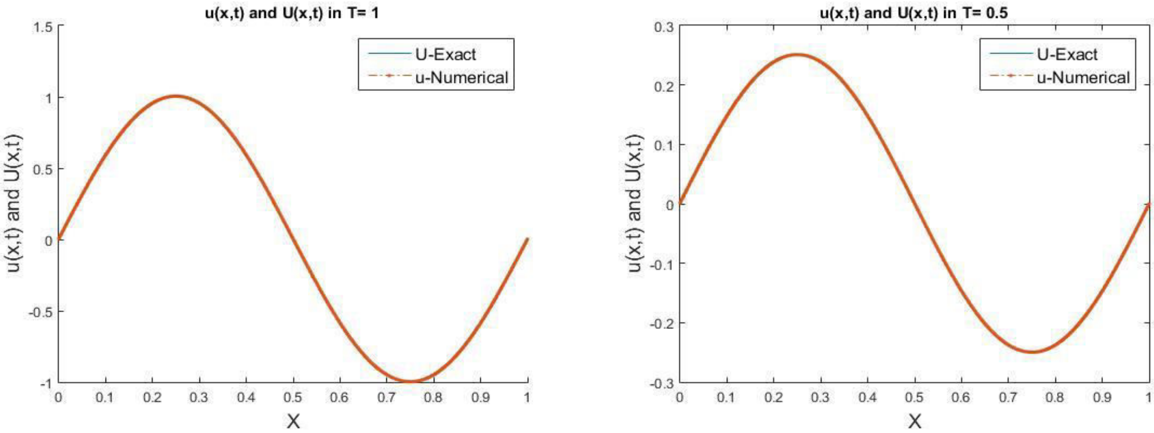

Fig. 3: Here result of analytical and approximate solution at $T = 0.5$, $T = 1$ for $\Delta x = 2^{-10}$ and $\Delta t = 2^{-7}$ at different x_S is shown.

CONCLUSION:

In this work, a numerical method based on the finite-difference approach is provided for solution of fractional-time diffusion equation, using the Neumann and Robin Boundary Conditions. The time derivative, meaning Caputo, is described of the α order. It has been concluded that by stability analysis of the problem, applied method is unconditionally stable, also the numerical analysis of the problem led us to conclusion, that numerical answers have very good compliance with exact answer of the problem. Moreover, this method seems simple to implement and also requires relatively little memory meanwhile benefiting from the proper performance, which can be mentioned as one of its advantages. The method can be easily extended to solve fractional PDEs with higher dimensions.

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In this literature, the Caputo temporal-fractional diffusion equation for different values of M and N is evaluated and **Table 1** lists the error values L_2 and L_{max} for varying values of $\Delta t, \Delta x$ for $\alpha = 0.5$. According to output of the problem, the error value decreases with the increased size of temporal and spatial meshes. However, variation of changes in the spatial meshes on the performance of the model seems to be higher, therefore the results reveal very good consistency between analytical and approximate solutions.

Table 1: The error values of L_2 and L_{max} are shown for various values of Δt, Δx for $\alpha = 0.5$ and $x = 0.5$.

Δx	Δt	L_2	L_{max}
2^{-7}	2^{-7}	1.3e-03	3e-03
2^{-8}	2^{-7}	6.73e-04	1.5e-03
2^{-10}	2^{-7}	1.89e-04	3.82e-04
2^{-7}	2^{-8}	7.7e-04	1.8e-03
2^{-7}	2^{-10}	2.98e-04	7.48e-04

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CONFLICTS OF INTEREST:

This research is contributed by all authors and no potential conflict of interest to publish it.

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