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Research article

Development and Analysis of Optimized Numerical Scheme for Three-Dimensional Linear Time-Fractional Diffusion Equations

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Abstract

In this paper, an optimized numerical method for solving time-fractional diffusion equations in three-dimensional space is proposed. Fractional-order differential equations can model complex physical processes with memory effects more accurately than differential equations with integer order derivatives. On the other hand, numerical solutions of this type of problem are usually challenging due to the existence of a singularity near the initial time. In the proposed method, in order to overcome this issue, the $L1$ formula has been used on a graded mesh to maintain the accuracy of calculations near the initial time. Also, a fourth-order compact operator has been used to discretize the Laplace operator in three-dimensional space. Stability and convergence analyses show that this method has a convergence order proportional to the grading parameter in time and a fourth-order convergence order in space. The obtained results from numerical simulations confirm the high accuracy of the proposed method and the efficiency of the optimal selection of the scaling parameter in achieving the suitable convergence order, even in the presence of initial singularities.

Keywords: Time-fractional diffusion equation, Graded mesh, Compact finite difference scheme, Stability and convergence analysis, Three-dimensional diffusion equation.

Mathematics Subject Classification (2020): 65M06, 65M12

1 Introduction

In recent decades, fractional differential equations (FDEs) have attracted the attention of many researchers due to their ability to accurately model complex physical processes with memory effects and heritable properties, and several numerical methods have been proposed for fractional differential problems in the literature [1–9]. Unlike classical integer-order calculus, fractional derivatives provide a powerful framework for describing anomalous diffusion, control theory, bioengineering, general transport theory, viscoelasticity, and signal processing. [10–16]. Solving high-dimensional fractional models analytically is often impossible or leads to complex series solutions that are difficult to evaluate. As a result, the development of efficient, rigorous and numerical algorithms is of great importance. Many researchers have proposed numerical methods for solving the time fractional diffusion equation. Some recent method poposed by researchers for TDFE are as follows. A Galerkin method based on the reproducing kernel particle method is proposed for the timefractional modified anomalous subdiffusion model of distributedorder [17]. A combination of the spectral element method and L1 formula on graded meshes is proposed for the time fractional diffusion equation [18]. A method based on the Galerkin Legendre spectral method is proposed for two-dimensional TFDE with delay [19]. An adopted spectral tau methodbased on the seventh-kind Chebyshev polynomials is applied for TFDE [20]. An explicit ChebyshevGalerkin scheme for the TFDE is proposed [21].

In this paper, we develop the numerical solution of the following three-dimensional linear time-fractional diffusion problem:

$$ {}^{C}\mathscr{D}^{\delta}\phi(\mathbf{x},t) = \Delta\phi(\mathbf{x},t) + f(\mathbf{x}), \quad \mathbf{x}\in\Omega, \quad t\in(0,T], \tag{1} $$

where

$$ \mathbf{x} = (x_1,x_2,x_3), \quad \Omega = (a,b)\times(c,d)\times(e,f), \quad J=(0,T], \quad 0<\delta<1, $$

and Δ is the three-dimensional Laplacian operator defined by

$$ \Delta\phi = \frac{\partial^2\phi}{\partial x_1^2} + \frac{\partial^2\phi}{\partial x_2^2} + \frac{\partial^2\phi}{\partial x_3^2}. $$

The initial and boundary conditions are given by

$$ \begin{cases} \phi(\mathbf{x},t) = 0, & \mathbf{x}\in\partial\Omega, \quad t\in J, \\ \phi(\mathbf{x},0) = \phi_0(\mathbf{x}), & \mathbf{x}\in\bar{\Omega} = \Omega\cup\partial\Omega, \end{cases} \tag{2} $$

where $\partial\Omega$ is the boundary of Ω.

One of the most widely used techniques for time discretization of Caputo's fractional derivative is the $L1$ scheme [11,18]. However, it is well known that the solutions of time fractional diffusion equations (TFDEs) usually exhibit a singularity near the initial time $t=0$, where the derivatives of the solution may explode even if the initial data are smooth [10].

Stynes et al. in [10] used a nonuniform or graded grid scheme to discretize fractional-order time derivatives and investigated the effect of graded grids on the convergence order of the method.

To overcome the singularity near the initial time, the use of graded meshes could be useful. This technique aggregates more points near the origin to effectively represent the unique behavior of the solution [22]. Researchers have successfully used graded grids to solve time-dependent partial integro-differential equations involving Riemann-Liouville fractional integrals, weakly singular Volterra integral equations and time-fractional nonlinear partial differential equations [23–26]. In [27], authors have shown that using graded grids for weakly singular Volterra integral equations produces more accurate results than uniform grids. In this paper, a combination of graded meshes and compact operators for 3D time-fractional diffusion equations using is explored. We propose an optimized numerical scheme for Eq. (1). The temporal derivative is approximated using the $L1$ formula on a graded mesh to handle initial singularities, while the spatial Laplacian is treated with a fourth-order compact finite difference operator. To prove the efficiency and accuracy of the proposed method, several numerical simulations are presented. The numerical results show that the optimal choice of the scaling parameter r achieves second-order time accuracy even in the presence of singular points near the initial time.

The main contributions of this work are as follows:

- We develop an efficient numerical scheme that achieves $\min\{r\delta, 2-\delta\}$ convergence in time and fourth-order convergence in space for three-dimensional time-dependent fractional differential equations.
- A rigorous stability and convergence analysis is presented.
- Numerical simulations are conducted to verify the analytical results and show the impact of the choice of the scaling parameter r to maintain accuracy.

The rest of the paper is organized as follows. Section 2 describes the construction of the proposed numerical scheme. The stability and convergence analysis of the optimized numerical scheme is presented in Section 3. In Section 4, numerical results are presented to validate the theoretical findings, and finally, concluding remarks are given in Section 5.

2 Optimized Numerical Scheme

Let N be a positive integer and consider a graded temporal mesh defined by

$$t_n = (n\Delta t)^r, \quad n = 0, 1, 2, \ldots, N,$$

where the uniform step in the graded scale is

$$\Delta t = \frac{T^{1/r}}{N}, \quad r \geq 1,$$

and $\Delta t_n = t_n - t_{n-1}$ denotes the size of the subinterval

$$I_n = [t_{n-1}, t_n], \quad 1 \leq n \leq N.$$

Let $0 < \delta < 1$ and $\{\phi^n\}_{n=0}^N$ be a sequence of functions defined on Ω. The $L1$-approximation for the Caputo fractional derivative at $t = t_n$ is defined as [10]

$$D_N^\delta \phi^n = \frac{d_{n,1}}{\Gamma(2-\delta)}\phi^n - \frac{d_{n,n}}{\Gamma(2-\delta)}\phi^0 + \frac{1}{\Gamma(2-\delta)}\sum_{k=1}^{n-1}(d_{n,k+1} - d_{n,k})\,\phi^{n-k}, \tag{3}$$

where the coefficients $d_{n,k}$ are given by

$$d_{n,k} = \frac{(t_n - t_{n-k})^{1-\delta} - (t_n - t_{n-k+1})^{1-\delta}}{\Delta t_{n-k+1}}, \quad 1 \leq k \leq n, \tag{4}$$

In particular,

$$d_{n,1} = \Delta t_n^{-\delta}.$$

Suppose that $\phi \in C[0,T] \cap C^2(0,T]$ and assume a constant C exists such that

$$|\phi^{(s)}(t)| \leq C\big(1 + t^{\delta - s}\big), \quad 0 < t \leq T,\ s = 0, 1, 2, \tag{5}$$

The local truncation error $(R_t)^n = {}^C\mathscr{D}^\delta \phi(t_n) - D_N^\delta \phi^n$ satisfies the inequality [10]

$$|(R_t)^n| \leq CN^{-\min\{r\delta, 2-\delta\}},\ n = 1, 2, \cdots, N,$$

Let M_1, M_2, and M_3 be three positive integers, and define the spatial step sizes

$$h_1 = \frac{b-a}{M_1}, \quad h_2 = \frac{d-c}{M_2}, \quad h_3 = \frac{f-e}{M_3}.$$

The corresponding spatial grid points are

$$\begin{aligned} x_{1,i} &= a + ih_1, \quad i = 0, 1, \ldots, M_1, \\ x_{2,j} &= c + jh_2, \quad j = 0, 1, \ldots, M_2, \\ x_{3,k} &= e + kh_3, \quad k = 0, 1, \ldots, M_3. \end{aligned}$$

We further define the following sets:

$$\begin{aligned} \overline{\Omega}_{h_1,h_2,h_3} &= \{\mathbf{x}_{ijk} = (x_{1,i}, x_{2,j}, x_{3,k}) \mid 0 \leq i \leq M_1,\ 0 \leq j \leq M_2,\ 0 \leq k \leq M_3\}, \\ \Omega_{h_1,h_2,h_3} &= \overline{\Omega}_{h_1,h_2,h_3} \cap \Omega, \\ \partial\Omega_{h_1,h_2,h_3} &= \overline{\Omega}_{h_1,h_2,h_3} \cap \partial\Omega. \end{aligned}$$

For a grid function

$$\phi = \{\phi_{i,j,k} = \phi(x_{1,i}, x_{2,j}, x_{3,k}) \mid (x_{1,i}, x_{2,j}, x_{3,k}) \in \overline{\Omega}_{h_1,h_2,h_3}\},$$

we define the standard second-order finite difference operators in each coordinate direction:

$$\begin{aligned}
\delta_{x_1}^2 \phi_{i,j,k} &= \frac{\phi_{i+1,j,k} - 2\phi_{i,j,k} + \phi_{i-1,j,k}}{h_1^2}, && 1 \le i \le M_1 - 1,\ 0 \le j \le M_2,\ 0 \le k \le M_3,\\
\delta_{x_2}^2 \phi_{i,j,k} &= \frac{\phi_{i,j+1,k} - 2\phi_{i,j,k} + \phi_{i,j-1,k}}{h_2^2}, && 1 \le j \le M_2 - 1,\ 0 \le i \le M_1,\ 0 \le k \le M_3,\\
\delta_{x_3}^2 \phi_{i,j,k} &= \frac{\phi_{i,j,k+1} - 2\phi_{i,j,k} + \phi_{i,j,k-1}}{h_3^2}, && 1 \le k \le M_3 - 1,\ 0 \le i \le M_1,\ 0 \le j \le M_2.
\end{aligned}$$

The following modified operators $\mathscr{L}_m$ $(m = 1,2,3)$ are defined to incorporate fourth-order compact corrections in the interior [11]:

$$\mathscr{L}_1 \phi_{i,j,k} = \begin{cases} \left(1 + \frac{1}{12} h_1^2 \delta_{x_1}^2\right) \phi_{i,j,k}, & 1 \le i \le M_1 - 1,\\ \phi_{i,j,k}, & i = 0, M_1, \end{cases} \qquad \mathscr{L}_2 \phi_{i,j,k} = \begin{cases} \left(1 + \frac{1}{12} h_2^2 \delta_{x_2}^2\right) \phi_{i,j,k}, & 1 \le j \le M_2 - 1,\\ \phi_{i,j,k}, & j = 0, M_2, \end{cases}$$

$$\mathscr{L}_3 \phi_{i,j,k} = \begin{cases} \left(1 + \frac{1}{12} h_3^2 \delta_{x_3}^2\right) \phi_{i,j,k}, & 1 \le k \le M_3 - 1,\\ \phi_{i,j,k}, & k = 0, M_3. \end{cases}$$

If $\phi(\mathbf{x}) \in C^{6,6,6}_{x_1,x_2,x_3}((a,b)\times(c,d)\times(e,f))$, then for $m = 1,2,3$, we have [11]:

$$\mathscr{L}_m \frac{\partial^2 \phi_{i,j,k}}{\partial x_m^2} = \delta_{x_m}^2 \phi_{i,j,k} + O(h_m^4).$$

We consider (1) at the mesh point $(\mathbf{x}_{ijk}, t_n)$ for $1 \le n \le N$, $1 \le i \le M_1 - 1$, $1 \le j \le M_2 - 1$ and $1 \le k \le M_3 - 1$, then we have

$${}^{C}\mathscr{D}^{\delta} \phi_{i,j,k}^n = \Delta \phi_{i,j,k}^n + f_{i,j,k}^n,\ 1 \le n \le N, 1 \le i \le M_1 - 1, 1 \le j \le M_2 - 1, 1 \le k \le M_3 - 1, \tag{6}$$

$$\phi_{i,j,k}^0 = (\phi_0)_{i,j,k},\ 0 \le i \le M_1,\ 0 \le j \le M_2,\ 0 \le k \le M_3, \tag{7}$$

$$\phi_{i,j,k}^n = 0,\ i = 0, M_1,\ j = 0, M_2,\ k = 0, M_3,\ 0 \le n \le N, \tag{8}$$

where $\phi_{i,j,k}^n = u(\mathbf{x}_{ij}, t_n)$.
By substituting $\phi_{i,j,k}^n$ with its numerical approximation $\Phi_{i,j,k}^n$, we derive the following linearized finite difference scheme:

$$\begin{aligned}
D_N^{\delta} \mathscr{L}_1 \mathscr{L}_2 \mathscr{L}_3 \Phi_{i,j,k}^n &= \mathscr{L}_2 \mathscr{L}_3 \delta_{x_1}^2 \Phi_{i,j,k}^n + \mathscr{L}_1 \mathscr{L}_3 \delta_{x_2}^2 \Phi_{i,j,k}^n + \mathscr{L}_1 \mathscr{L}_2 \delta_{x_3}^2 \Phi_{i,j,k}^n + \mathscr{L}_1 \mathscr{L}_2 \mathscr{L}_3 f_{i,j,k}^n,\\
&\quad 1 \le n \le N,\ 1 \le i \le M_1 - 1,\ 1 \le j \le M_2 - 1,\ 1 \le k \le M_3 - 1,
\end{aligned} \tag{9}$$

$$\Phi_{i,j,k}^0 = (\phi_0)_{i,j,k}, \quad 0 \le i \le M_1,\ 0 \le j \le M_2,\ 0 \le k \le M_3, \tag{10}$$

$$\Phi_{i,j,k}^n = 0, \quad i \in \{0, M_1\} \text{ or } j \in \{0, M_2\} \text{ or } k \in \{0, M_3\}, \quad 0 \le n \le N. \tag{11}$$

3 Stability and Convergence Analysis

3.1 Stability Analysis

To analyze the stability of the scheme (9)–(11), we introduce $\widetilde{\Phi}_{i,j,k}^n$ as the numerical solution obtained from (9)–(11) in the presence of perturbations in the source term and initial data

$$\begin{aligned}
&D_N^{\delta} \mathscr{L}_1 \mathscr{L}_2 \mathscr{L}_3 \widetilde{\Phi}_{i,j,k}^n = \mathscr{L}_2 \mathscr{L}_3 \delta_{x_1}^2 \widetilde{\Phi}_{i,j,k}^n + \mathscr{L}_1 \mathscr{L}_3 \delta_{x_2}^2 \widetilde{\Phi}_{i,j,k}^n + \mathscr{L}_1 \mathscr{L}_2 \delta_{x_3}^2 \widetilde{\Phi}_{i,j,k}^n + \mathscr{L}_1 \mathscr{L}_2 \mathscr{L}_3 f_{i,j,k}^n + h_{i,j,k}^n,\\
&1 \le n \le N,\ 1 \le i \le M_1 - 1,\ 1 \le j \le M_2 - 1,\ 1 \le k \le M_3 - 1,
\end{aligned} \tag{12}$$

$$\widetilde{\Phi}_{i,j,k}^0 = (\phi_0)_{i,j,k} + s_{i,j,k}, \qquad 0 \le i \le M_1,\ 0 \le j \le M_2,\ 0 \le k \le M_3, \tag{13}$$

$$\widetilde{\Phi}_{i,j,k}^n = 0, \qquad i = 0, M_1,\ j = 0, M_2,,\ k = 0, M_3,\ 0 \le n \le N. \tag{14}$$

Define the perturbation errors by

$$E^n_{i,j,k} = \widetilde{\Phi}^n_{i,j,k} - \Phi^n_{i,j,k}.$$

By subtracting the original scheme (9)–(11) from the perturbed system (12)–(14), we obtain the corresponding error equations governing $E^n_{i,j,k}$:

$$\begin{aligned} D^\delta_N \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3 E^n_{i,j,k} &= \mathscr{L}_2\mathscr{L}_3\delta^2_{x_1}E^n_{i,j,k} + \mathscr{L}_1\mathscr{L}_3\delta^2_{x_2}E^n_{i,j,k} + \mathscr{L}_1\mathscr{L}_2\delta^2_{x_3}E^n_{i,j,k} \\ &+ h^n_{i,j,k}, \quad 1 \le n \le N,\ 1 \le i \le M_1 - 1,\ 1 \le j \le M_2 - 1,,\ 1 \le k \le M_3 - 1, \end{aligned} \tag{15}$$

$$E^0_{i,j,k} = s^0_{i,j,k}, \quad 0 \le i \le M_1,\ 0 \le j \le M_2,\ 0 \le k \le M_3, \tag{16}$$

$$E^n_{i,j,k} = 0, \quad i = 0, M_1,\ j = 0, M_2,\ k = 0, M_3,\ 0 \le n \le N. \tag{17}$$

Lemma 1. *The proposed finite difference scheme is stable, and we have*

$$\|E^n\| \le C\left(\|s^0\| + \max_{1\le j\le n}\|h^j\|\right),\ 1 \le n \le N, \tag{18}$$

where C is the positive constant and

$$E^n = \{E^n_{i,j,k}\}, h^n = \{h^n_{i,j,k}\}, s^0 = \{s^0_{i,j,k}\}.$$

Proof. Suppose that

$$\Phi^n = \{\Phi^n_{i,j,k}\} \quad \text{and} \quad \widetilde{\Phi}^n = \{\widetilde{\Phi}^n_{i,j,k}\}.$$

Taking the inner product of (15) with $\mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n$, we obtain

$$\langle D^\delta_N \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle - \langle \mathscr{L}_2\mathscr{L}_3\delta^2_{x_1}E^n + \mathscr{L}_1\mathscr{L}_3\delta^2_{x_2}E^n + \mathscr{L}_1\mathscr{L}_2\delta^2_{x_3}E^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle = \langle h^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle, 1 \le n \le N. \tag{19}$$

We have

$$\langle h^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle \le \|h^n\|\|E^n\|. \tag{20}$$

We also know

$$-\langle \mathscr{L}_2\mathscr{L}_3\delta^2_{x_1}E^n + \mathscr{L}_1\mathscr{L}_3\delta^2_{x_2}E^n + \mathscr{L}_1\mathscr{L}_2\delta^2_{x_3}E^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle \ge 0. \tag{21}$$

After applying Theorem [22, Theorem 2.1], we have

$$\frac{1}{2}D^\delta_N\|\mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\|^2 \le \langle D^\delta_N \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle - \langle \mathscr{L}_2\mathscr{L}_3\delta^2_{x_1}E^n + \mathscr{L}_1\mathscr{L}_3\delta^2_{x_2}E^n + \mathscr{L}_1\mathscr{L}_2\delta^2_{x_3}E^n, \mathscr{L}_1\mathscr{L}_2\mathscr{L}_3E^n\rangle, \tag{22}$$

Combining (19)–(22), we get

$$D^\delta_N\|E^n\|^2 \le C\|h^n\|\|E^n\|. \tag{23}$$

Now, using [22, Lemma 2.2], it follows that

$$\|E^n\| \le C\left(\|s^0\| + \max_{1\le j\le n}\|h^j\|\right),\ 1 \le n \le N. \tag{24}$$

□

3.2 Convergence Analysis

By applying (6)–(8), we obtain

$$\begin{aligned} D_N^{\delta}\mathscr{L}_1\mathscr{L}_2\mathscr{L}_3\phi_{i,j,k}^n &= \mathscr{L}_2\mathscr{L}_3\delta_{x_1}^2\phi_{i,j,k}^n+\mathscr{L}_1\mathscr{L}_3\delta_{x_2}^2\phi_{i,j,k}^n+\mathscr{L}_1\mathscr{L}_2\delta_{x_3}^2\phi_{i,j,k}^n+(R_{t,\mathbf{x}})_{i,j,k}^n, \\ &\qquad 1\le n\le N,\ 1\le i\le M_1-1,\ 1\le j\le M_2-1,,\ 1\le k\le M_3-1, \end{aligned} \tag{25}$$

$$\phi_{i,j,k}^0 = (\phi_0)_{i,j,k},\quad 0\le i\le M_1,\ 0\le j\le M_2,\ 0\le k\le M_3, \tag{26}$$

$$\phi_{i,j,k}^n = 0,\quad i=0,M_1,\ j=0,M_2,,\ k=0,M_3,\ 0\le n\le N. \tag{27}$$

where

$$(R_{t,\mathbf{x}})_{i,j,k}^n = O(N^{-\min\{r\delta,2-\delta\}}+h_1^4+h_2^4+h_3^4).$$

Let us define the error as

$$e_{i,j,k}^n = \phi_{i,j,k}^n-\Phi_{i,j,k}^n.$$

By subtracting equations (25)–(27) from (9)–(11), we obtain

$$\begin{aligned} D_N^{\delta}\mathscr{L}_1\mathscr{L}_2\mathscr{L}_3 e_{i,j,k}^n &= \mathscr{L}_2\mathscr{L}_3\delta_{x_1}^2 e_{i,j,k}^n+\mathscr{L}_1\mathscr{L}_3\delta_{x_2}^2 e_{i,j,k}^n+\mathscr{L}_1\mathscr{L}_2\delta_{x_3}^2 e_{i,j,k}^n+(R_{t,\mathbf{x}})_{i,j,k}^n, \\ &\qquad 1\le n\le N,\ 1\le i\le M_1-1,\ 1\le j\le M_2-1,,\ 1\le k\le M_3-1, \end{aligned} \tag{28}$$

$$e_{i,j,k}^0 = 0,\quad 0\le i\le M_1,\ 0\le j\le M_2,\ 0\le k\le M_3, \tag{29}$$

$$e_{i,j,k}^n = 0,\quad i=0,M_1,\ j=0,M_2,,\ k=0,M_3,\ 0\le n\le N. \tag{30}$$

Theorem 1. *Let $\phi\in C[0,T]\cap C^2(0,T]$, and suppose that there exists a positive constant C such that*

$$|\phi^{(m)}(t)|\le C\big(1+t^{\delta-m}\big),\quad m=0,1,2,\quad 0<t\le T. \tag{31}$$

Then, there exists a positive integer N_* such that for all $N\ge N_*$, the following error estimate holds:

$$\|e^n\|\le C\left(N^{-\min\{r\delta,2-\delta\}}+h_1^4+h_2^4+h_3^4\right),\quad 1\le n\le N, \tag{32}$$

where C is a positive constant independent of h_1, h_2, h_3, and N and

$$e^n=\{e_{i,j,k}^n\}.$$

Proof. This theorem can be proved in a similar manner to Lemma 1. □

4 Numerical Example

To verify the performance and reliability of the high-order numerical scheme, we perform a detailed numerical experiment. All simulations are executed on a Windows 10 laptop running MATLAB 2021a, featuring a six-core Intel Core i7-10750H processor with a maximum clock speed of 5.00 GHz and 16 GB of DDR4 memory. In this study, a representative example is considered to validate the theoretical findings. We set $M_1=M_2=M_3=M$. At the final time level $t=T$, let Φ^N and ϕ^N represent the vector forms of the discrete approximation $\{\Phi_{i,j}^N\}$ and the exact values $\{\phi(\mathbf{x}_{ijk},T)\}$, respectively, for $1\le i,j,k\le M-1$.
The discrete error at time T is measured in the maximum norm as

$$E(h,N)=\left\|\Phi^N-\phi^N\right\|_\infty=\max_{1\le i,j,k\le M-1}\left|\Phi_{i,j,k}^N-\phi(\mathbf{x}_{ijk},T)\right|.$$

Example 1. In this example, the forcing term f is determined in such a way that the exact analytical solution takes the form

$$\phi(\mathbf{x},t) = t^{\delta} \sin(\pi x_1)\sin(\pi x_2)\sin(\pi x_3)\,,\ \mathbf{x} \in (0,1)^3,\ t \in (0,1]. \tag{33}$$

Tables 1 and 2 report the maximum error and the convergence rate in the temporal direction at $T = 1$ for various values of N and different choices of the parameter r. Since $\frac{2-\delta}{\delta} > 1$, the optimal value of the parameter is $r_{\text{opt}} = \frac{2-\delta}{\delta}$.

Tables 3 and 4 report the maximum error and the numerical convergence rate at $T = 1$ for different spatial step sizes h. The observed convergence rate are close to the theoretical value, which confirms the accuracy of the proposed numerical scheme in the spatial direction. If one chooses $r < \frac{2-\delta}{\delta}$, the temporal convergence rate is limited to $r\delta$, which grows with r but stays below $2-\delta$. Taking $r \geq \frac{2-\delta}{\delta}$ saturates the bound and allows the scheme to achieve the maximum possible order $2-\delta$. Thus, the optimal value that gives the highest accuracy without unnecessary mesh grading is $r_{\text{opt}} = \frac{2-\delta}{\delta}$.

Table 1. Error and convergence rate (CR) in the temporal direction at $T = 1$ for $h = 1/2^4$ with $\delta = 0.5$.

N	$r_{\text{opt}} = \frac{2-\delta}{\delta}$		$r = \frac{3(2-\delta)}{\delta}$		$r = \frac{4(2-\delta)}{\delta}$	
	$Error$	CR	$Error$	CR	$Error$	CR
25	3.53770e-04	...	5.26750e-04	...	5.26750e-04	...
50	1.27215e-04	1.4755	1.93757e-04	1.4429	1.93757e-04	1.4429
100	4.26456e-05	1.5768	6.75258e-05	1.5207	6.75258e-05	1.5207
200	9.44675e-06	2.1745	2.15885e-05	1.6452	3.07312e-05	1.1357

Table 2. Error and convergence rate (CR) in the temporal direction at $T = 1$ for $h = 1/2^4$ with $\delta = 0.9$.

N	$r_{\text{opt}} = \frac{2-\delta}{\delta}$		$r = \frac{2(2-\delta)}{\delta}$		$r = \frac{3(2-\delta)}{\delta}$	
	$Error$	CR	$Error$	CR	$Error$	CR
25	4.51607e-05	...	9.91952e-05	...	1.55446e-04	...
50	1.76766e-05	1.3532	4.29682e-05	1.2070	6.95508e-05	1.1603
100	5.00562e-06	1.8202	1.68207e-05	1.3530	2.93063e-05	1.2469
200	1.86139e-06	1.4272	6.17823e-06	1.4450	9.98745e-06	1.5530

Table 3. $Error$ and convergence rate CR in the spatial direction, at $T = 1$ with $N = 200$ for $r_{\text{opt}} = \frac{2-\delta}{\delta}$.

h	$\delta = 0.6$		$\delta = 0.8$	
	$Error$	CR	$Error$	CR
1/2	2.72216e-02	—	2.71764e-02	—
$1/2^2$	1.57224e-03	4.1139	1.56822e-03	4.1152
$1/2^3$	9.22532e-05	4.0911	9.05362e-05	4.1145
$1/2^4$	5.68546e-06	4.0202	5.57891e-06	4.0204

5 Conclusion

In this paper, an efficient numerical method for solving three-dimensional time-fractional diffusion equations has been presented. The method is a combination of a graded mesh scheme for discretization in the time direction, and a fourth-order compact operator is utilized

Table 4. $Error$ and convergence rate CR in the spatial direction, at $T=1$ with $N=200$ for $r_{\text{opt}}=\frac{2-\delta}{\delta}$.

h	$\delta=0.7$		$\delta=0.95$	
	$Error$	CR	$Error$	CR
1/2	2.72026e-02	—	2.71266e-02	—
$1/2^2$	1.57026e-03	4.1147	1.56797e-03	4.1127
$1/2^3$	9.12243e-05	4.1054	9.30538e-05	4.0747
$1/2^4$	5.55712e-06	4.0370	5.39159e-06	4.1093

for discretization in the space direction. The use of a nonuniform time step size allowed us to handle the singularity of the solution near the initial time and to avoid the loss of accuracy due to the singularity. The convergence analysis and the presented numerical results showed that with the appropriate choice of the scaling parameter, second-order accuracy in time and fourth-order accuracy in space can be achieved. The stability of the method was mathematically proven, and the numerical examples provided are also in agreement with the theoretical analyses. Possible future research directions include extending this method to higher-dimensional problems and different types of fractional differential equations.

Data Availability

No data were used to support this study.

Conflicts of Interest

The author declares that there is no conflict of interest.

Ethical Considerations

The author has diligently addressed ethical concerns, such as informed consent, plagiarism, data fabrication, misconduct, falsification, double publication, redundancy, submission, and other related matters.

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