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A spatially second-order accurate implicit numerical method for the space and time fractional Bloch-Torrey equation

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Abstract In recent years, it has been found that many phenomena in engineering, physics, chemistry and other sciences can be described very successfully by models using mathematical tools from Fractional Calculus. Recently, a new space and time fractional Bloch-Torrey equation (ST-FBTE) has been proposed [13], and successfully applied to analyse diffusion images of human brain tissues to provide new insights for further investigations of tissue structures.

In this paper, we consider the ST-FBTE with a nonlinear source term on a finite domain in three-dimensions. The time and space derivatives in the ST-FBTE are replaced by the Caputo and the sequential Riesz fractional derivatives, respectively. Firstly, we propose a spatially second-order accurate implicit numerical method (INM) for the ST-FBTE whereby we discretize the Riesz fractional derivative using a fractional centered difference. Secondly, we prove that the implicit numerical method for the ST-FBTE is uniquely solvable, unconditionally stable and convergent, and the order of convergence

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of the implicit numerical method is $O(\tau^{2-\alpha}+\tau+h_x^2+h_y^2+h_z^2)$. Finally, some numerical results are presented to support our theoretical analysis.

Keywords Fractional Bloch-Torrey equation · Fractional Calculus · implicit numerical method · fractional centered difference · solvability · stability · convergence

1 Introduction

It is now well accepted that many phenomena in engineering, physics, chemistry and other sciences can be described very successfully by models that employ the theory of derivatives and integrals of fractional order [4,5,10,11, 18,20,22,28,29]. At present, fractional order equations have been applied to model dynamical systems in science and engineering [12,26]. These new fractional models are more adequate than the previously used integer order models [17], because fractional order derivatives and integrals enable the description of the memory and hereditary properties of different substances.

In physics, particularly when applied to diffusion, fractional order dynamics lead to an extension of Brownian motion to what is called anomalous diffusion [13]. Anomalous diffusion concerns the theory of diffusing particles in environments that are not locally homogeneous, including disorder that is not well-approximated by assuming a unified change in the diffusion constant. Such systems include diffusion in complicated structures such as brain tissue. Hall and Barrick [7] show that the usual manner to study the diffusive dynamics is to investigate the mean square displacement $\langle r^2(t)\rangle$ of the particles, namely

$$\langle r^2(t)\rangle \propto t^\alpha,\ t\to\infty, \tag{1}$$

where α is the anomalous diffusion exponent.

A very interesting and particular class of complex phenomena arises in the nuclear magnetic resonance (NMR) and magnetic resonance imaging (MRI) fields, and Fractional Calculus may help to express a physical meaning by utilizing the fractional derivative operator [14,15]. If the complex heterogeneous structure, such as spatial connectivity, can facilitate the movement of particles at a certain scale, fast motions may no longer obey the classical Fick's law and may indeed have a probability density function that follows a power-law. For example, if $C(x,t)$ represents the concentration of the diffusing species in one-dimension, then a space-time Riesz-Caputo fractional diffusion equation of the form

$${}_0^C D_t^\alpha C(x,t) = K_x \frac{\partial^\beta C(x,t)}{\partial |x|^\beta}, \tag{2}$$

emerges from Fick's first law in the continuity equation [6], where K_x is the generalized diffusion coefficint, ${}_0^C D_t^\alpha$ is the Caputo time fractional derivative of order α $(0<\alpha<1)$ with respect to t with starting point at $t=0$ defined as [17]:

$${}_0^C D_t^\alpha C(x,t) = \frac{1}{\Gamma(1-\alpha)}\int_0^t \frac{C'(x,\tau)}{(t-\tau)^\alpha}d\tau, \tag{3}$$

and $R_x^\beta = \frac{\partial^\beta}{\partial |x|^\beta}$ is the Riesz fractional derivative of order β $(1 < \beta \leq 2)$ with respect to x, which is defined in equation (5) below.

Recently, some authors have used Fractional Calculus to investigate the connection between fractional order dynamics and diffusion by solving the Bloch-Torrey equation [13,23,24]. They have demonstrated that a Fractional Calculus based diffusion model can be successfully applied to analyzing diffusion images of human brain tissues and provide new insights for further investigations of tissue structures. The following new diffusion model was proposed for solving the Bloch-Torrey equation using Fractional Calculus with respect to time and space [13]:

$$\tau^{\alpha-1}\ {}_0^C D_t^\alpha M_{xy}(\mathbf{r},t) = \lambda M_{xy}(\mathbf{r},t) + D\mu^{2(\beta-1)}\mathbf{R}^\beta M_{xy}(\mathbf{r},t), \tag{4}$$

where $\lambda = -i\gamma(\mathbf{r}\cdot\mathbf{G}(t))$, $\mathbf{r} = (x,y,z)$, $\mathbf{G}(t)$ is the magnetic field gradient, γ and D are the gyromagnetic ratio and the diffusion coefficient, respectively. In addition, $\mathbf{R}^\beta = (R_x^\beta + R_y^\beta + R_z^\beta)$ is a sequential Riesz fractional order operator in space [8]. $M_{xy}(\mathbf{r},t) = M_x(\mathbf{r},t) + iM_y(\mathbf{r},t)$, where $i = \sqrt{-1}$, comprises the transverse components of the magnetization; $\tau^{\alpha-1}$ and $\mu^{2(\beta-1)}$ are the fractional order time and space constants needed to preserve units, respectively $(0 < \alpha \leq 1$, and $1 < \beta \leq 2)$. The fractional order dynamics derived from the space fractional Bloch-Torrey equation can be used to fit the signal attenuation in diffusion-weighted images obtained from Sephadex gels, human articular cartilage and a human brain [13], and can also be used to analyse diffusion images of healthy human brain tissues in vivo at high b values up to 4700 sec/mm^2 (b is the degree of diffusion sensitization defined by the amplitude and the time course of the magnetic field gradient pulses used to encode molecular diffusion displacements [9]) [27].

Compared with the considerable work carried out on the theoretical analysis, relatively little work has been done on the numerical solution of (4). Magin et al. [13] derived the analytical solutions with fractional order dynamics in space (i.e., $\alpha = 1$, β an arbitrary real number, $1 < \beta \leq 2$) and time (i.e., $0 < \alpha < 1$, and $\beta = 2$), respectively. Yu et al. [24] derived an analytical solution for solving (4) using a fractional Laplacian based model and an effective implicit numerical method for solving (4) using a Riesz fractional based model. They also considered the stability and convergence of the implicit numerical method. However, due to the computational overheads necessary to perform the simulations for solving (4) in three dimensions, Yu et al. [24] presented a preliminary study based on a two-dimensional example to confirm their theoretical analysis. Yu et al. [23] proposed a fractional alternating direction implicit scheme to overcome the computational bottlenecks described in [24], they also proved the stability and convergence of the proposed method. However, the order of convergence in [23,24] is $O(\tau^{2-\alpha} + h_x + h_y + h_z)$ first order in space.

The Grünwald-Letnikov derivative approximation scheme of order $O(h)$ is generally used to approximate the Riesz fractional derivative [17,18,20,23,24, 29]. In order to obtain a better approximation, Ortigueira [16] defined the 'fractional centered derivative' and proved that the Riesz fractional derivative of an analytic function can be represented by the fractional centered derivative. Celik and Duman [3] used the fractional centered derivative to approximate the Riesz fractional derivative and applied the Crank-Nicolson method to a fractional diffusion equation that utilises the Riesz fractional derivative, and showed that the method is unconditionally stable and convergent with $O(h^2)$ accuracy. Yu et al. [25] derived an effective implicit numerical method for solving (4) in two-dimensions with a linear source term using the fractional centered derivative to approximate the Riesz fractional derivative. They also considered the stability and convergence of the implicit numerical method, however, they did not consider the method's solvability, and the order of convergence in [25] is $O(\tau^{2-\alpha}+\tau+h_x^2+h_y^2)$.

In this paper, we build upon the work in [25] and use a fractional centered derivative to approximate the Riesz fractional derivative, and propose a new effective implicit numerical method for the space and time fractional Bloch-Torrey equation (ST-FBTE) with a nonlinear source term with initial and boundary conditions on a finite domain in three-dimensions, and prove that the implicit numerical method for the ST-FBTE is uniquely solvable, unconditionally stable and convergent. The convergence order is $O(\tau^{2-\alpha}+\tau+h_x^2+h_y^2+h_z^2)$.

The remainder of this article is arranged as follows. Some mathematical preliminaries related to Fractional Calculus are introduced in section 2. In section 3, we propose a new effective implicit numerical method for the ST-FBTE. The solvability, stability and convergence of the implicit numerical method are investigated in sections 4, 5 and 6, respectively. Finally, some numerical results are presented to show that our new implicit numerical method can obtain second order space accuracy, which is $O(\tau^{2-\alpha}+\tau+h_x^2+h_y^2+h_z^2)$.

2 Preliminary knowledge

In this section, we give some preliminary information that is assumed throughout this paper.

Definition 1. [23] The Riesz fractional operator $\mathbf{R}^\beta$ for $n-1<\beta\le n$ on a finite domain $[0,L_1]\times[0,L_2]\times[0,L_3]$ is defined as

$$R_x^\beta C(x,y,z,t)=\frac{\partial^\beta C(x,y,z,t)}{\partial|x|^\beta}=-c_\beta({}_0D_x^\beta+{}_xD_{L_1}^\beta)C(x,y,z,t), \qquad (5)$$

where $c_\beta=\frac{1}{2\cos(\frac{\pi\beta}{2})}$, $\quad \beta\neq 1$,

$$ {}_0D_x^\beta C(x,y,z,t)=\frac{1}{\Gamma(n-\beta)}\frac{\partial^n}{\partial x^n}\int_0^x\frac{C(\xi,y,z,t)d_\xi}{(x-\xi)^{\beta+1-n}},$$

$$ {}_xD_{L_1}^\beta C(x,y,z,t)=\frac{(-1)^n}{\Gamma(n-\beta)}\frac{\partial^n}{\partial x^n}\int_x^{L_1}\frac{C(\xi,y,z,t)d_\xi}{(\xi-x)^{\beta+1-n}}.$$

Similarly, we can define the Riesz fractional derivatives $R_y^\beta C(x,y,z,t) = \frac{\partial^\beta C(x,y,z,t)}{\partial |y|^\beta}$ and $R_z^\beta C(x,y,z,t) = \frac{\partial^\beta C(x,y,z,t)}{\partial |z|^\beta}$ of order β $(1 < \beta \leq 2)$ with respect to y and z.

Now, we present our solution techniques for the ST-FBTE for a finite domain. Firstly, the ST-FBTE (4) can be rewritten as:

$$K_\alpha \, {}_0^C D_t^\alpha M_{xy}(\mathbf{r},t) = \lambda M_{xy}(\mathbf{r},t) + K_\beta \mathbf{R}^\beta M_{xy}(\mathbf{r},t), \tag{6}$$

where $K_\alpha = \tau^{\alpha-1}$ and $K_\beta = D\mu^{2(\beta-1)}$.

For the numerical solutions of the ST-FBTE, we equate real and imaginary components to express (6) as a coupled system of partial differential equations for the components M_x and M_y, namely

$$K_\alpha \, {}_0^C D_t^\alpha M_x(\mathbf{r},t) = K_\beta (\frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta}) M_x(\mathbf{r},t) + \lambda_G M_y(\mathbf{r},t), \tag{7}$$

$$K_\alpha \, {}_0^C D_t^\alpha M_y(\mathbf{r},t) = K_\beta (\frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta}) M_y(\mathbf{r},t) - \lambda_G M_x(\mathbf{r},t), \tag{8}$$

where $\lambda_G = \gamma(\mathbf{r} \cdot \mathbf{G}(t))$.

For convenience, (7) and (8) are decoupled, which is equivalent to solving

$$K_\alpha \, {}_0^C D_t^\alpha M(\mathbf{r},t) = K_\beta (\frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta}) M(\mathbf{r},t) + f(M,\mathbf{r},t), \tag{9}$$

where M can be either M_x or M_y, and $f(M,\mathbf{r},t) = \lambda_G M_y(\mathbf{r},t)$ if $M = M_x$, and $f(M,\mathbf{r},t) = -\lambda_G M_x(\mathbf{r},t)$ if $M = M_y$.

3 Implicit numerical method for the ST-FBTE

In this section, we propose a new implicit numerical method for the following space and time fractional Bloch-Torrey equation with initial and boundary conditions on a finite domain:

$$K_\alpha \, {}_0^C D_t^\alpha M(\mathbf{r},t) = K_\beta (\frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta}) M(\mathbf{r},t) + f(M,\mathbf{r},t), \tag{10}$$

$$M(\mathbf{r},0) = M_0(\mathbf{r}), \tag{11}$$

$$M(\mathbf{r},t)|_{\bar{\Omega}} = 0, \tag{12}$$

where $0 < \alpha \leq 1$, $1 < \beta \leq 2$, $0 < t \leq T$, $\mathbf{r} = (x,y,z) \in \Omega$, Ω is the finite rectangular region $[0,L_1] \times [0,L_2] \times [0,L_3]$, and $\bar{\Omega}$ is $\mathbb{R}^3 - \Omega$, the nonlinear source term $f(M,\mathbf{r},t)$ is assumed locally Lipschitz continuous.

Remark 1: [1,2] We say that $f: X \to X$ is globally Lipschitz continuous if for some $L > 0$, we have $\|f(u) - f(v)\| \leq L\|u - v\|$ for all $u,\ v \in X$, and is locally Lipschitz continuous, if the latter holds for $\|u\|,\ \|v\| \leq M$ with $L = L(M)$ for any $M > 0$.

Baeumer et al. [1,2] showed how to solve nonlinear reaction-diffusion equations of type (10) by an operator splitting method when the abstract function f is only locally Lipschitz (see [1,2,21]).

Thus, we assume that for all $k = 1, 2, \cdots, N$, $\|u(x, y, z, t_k)\|$, $\|v(x, y, z, t_k)\| \leq M_k$ with a constant $M_k > 0$ for any $\mathbf{r} = (x, y, z) \in \Omega$, we have

$$\begin{aligned} \|f(u(x, y, z, t_k)) - f(v(x, y, z, t_k))\| &\leq L(M_k)\|u(x, y, z, t_k) - v(x, y, z, t_k)\| \\ &= L_k\|u(x, y, z, t_k) - v(x, y, z, t_k)\|, \quad (13) \end{aligned}$$

where we have defined $L_k = L(M_k)$ and $L_{\max} = \max\limits_{0\leq k\leq N} L_k$.

Let $h_x = L_1/N_1, h_y = L_2/N_2, h_z = L_3/N_3$, and $\tau = T/N$ be the spatial and time steps, respectively. For $i, j, k \in \mathbb{N}$ and $n \in \mathbb{N}$, we denote the exact and numerical solutions $M(\mathbf{r}, t)$ at a point (x_i, y_j, z_k) at the moment of time t_n as $m(x_i, y_j, z_k, t_n)$ and $m_{i,j,k}^n$, respectively. Similar notations for $f(M(x_i, y_j, z_k, t_n), x_i, y_j, z_k, t_n)$ and $f_{i,j,k}^n$.

Firstly, utilizing the discrete scheme in [18], we can discretize the Caputo time fractional derivative of $m(x_i, y_j, z_k, t_{n+1})$ as

$$\begin{aligned} {}_0^C D_t^\alpha m(x_i, y_j, z_k, t_{n+1}) = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{l=0}^{n} b_l [m(x_i, y_j, z_k, t_{n+1-l}) \\ - m_(x_i, y_j, z_k, t_{n-l})] + O(\tau^{2-\alpha}), \quad (14) \end{aligned}$$

where $b_l = (l+1)^{1-\alpha} - l^{1-\alpha}$, $l = 0, 1, \cdots, N$.

Secondly, adopting the fractional centered difference scheme in [3], we can discretize the Riesz fractional derivative as

$$\frac{\partial^\beta}{\partial|x|^\beta} m(x_i, y_j, z_k, t_{n+1}) = -\frac{1}{h_x^\beta} \sum_{p=-N_1+i}^{i} \omega_p m(x_{i-p}, y_j, z_k, t_{n+1}) + O(h_x^2), \quad (15)$$

where the coefficients ω_p are defined by

$$\omega_p = \frac{(-1)^p \Gamma(\beta+1)}{\Gamma(\frac{\beta}{2} - p + 1)\Gamma(\frac{\beta}{2} + p + 1)}, p = 0, \mp 1, \mp 2, \cdots. \quad (16)$$

Similarly,

$$\frac{\partial^\beta}{\partial|y|^\beta} m(x_i, y_j, z_k, t_{n+1}) = -\frac{1}{h_y^\beta} \sum_{q=-N_2+j}^{j} \omega_q m(x_i, y_{j-q}, z_k, t_{n+1}) + O(h_y^2), \quad (17)$$

$$\frac{\partial^\beta}{\partial|z|^\beta} m(x_i, y_j, z_k, t_{n+1}) = -\frac{1}{h_z^\beta} \sum_{r=-N_3+k}^{k} \omega_r m(x_i, y_j, z_{k-r}, t_{n+1}) + O(h_z^2). \quad (18)$$

The nonlinear source term can be treated either explicitly or implicitly. In this paper, we use an explicit method and evaluate the nonlinear source term at the previous time step:

$$f_{i,j,k}^{n+1} = f_{i,j,k}^n + O(\tau). \quad (19)$$

In this way, we avoid solving a nonlinear system at each time step and obtain an unconditionally stable and convergent numerical scheme, as shown in sections 5 and 6. However, the shortcoming of the explicit method is that it generates additional temporal error, as shown in (19).

Then we can obtain the implicit numerical scheme:

$$\frac{K_\alpha \tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{l=0}^{n} b_l (m_{i,j,k}^{n+1-l} - m_{i,j,k}^{n-l}) = -K_\beta \Big(\frac{1}{h_x^\beta} \sum_{p=-N_1+i}^{i} \omega_p m_{i-p,j,k}^{n+1} + \frac{1}{h_y^\beta} \sum_{q=-N_2+j}^{j} \omega_q m_{i,j-q,k}^{n+1} + \frac{1}{h_z^\beta} \sum_{r=-N_3+k}^{k} \omega_r m_{i,j,k-r}^{n+1} \Big) + f_{i,j,k}^{n}. \tag{20}$$

Thus, we have the following implicit difference approximation:

$$m_{i,j,k}^{n+1} + \mu_1 \sum_{p=-N_1+i}^{i} \omega_p m_{i-p,j,k}^{n+1} + \mu_2 \sum_{q=-N_2+j}^{j} \omega_q m_{i,j-q,k}^{n+1} + \mu_3 \sum_{r=-N_3+k}^{k} \omega_r m_{i,j,k-r}^{n+1} = \sum_{l=0}^{n-1} (b_l - b_{l+1}) m_{i,j,k}^{n-l} + b_n m_{i,j,k}^{0} + \mu_0 f_{i,j,k}^{n}, \tag{21}$$
$$i = 1, 2, \cdots, N_1 - 1, j = 1, 2, \cdots, N_2 - 1, k = 1, 2, \cdots, N_3 - 1,$$

with

$$m_{i,j,k}^{0} = g_{i,j,k} = g(x_i, y_j, z_k),$$
$$m_{0,j,k}^{n+1} = m_{N_1,j,k}^{n+1} = m_{i,0,k}^{n+1} = m_{i,N_2,k}^{n+1} = m_{i,j,0}^{n+1} = m_{i,j,N_3}^{n+1} = 0,$$
$$(i = 0, 1, \cdots, N_1, j = 0, 1, \cdots, N_2, k = 0, 1, \cdots, N_3)$$

where $\mu_0 = \frac{\tau^\alpha \Gamma(2-\alpha)}{K_\alpha}$, $\mu_1 = \frac{K_\beta \tau^\alpha \Gamma(2-\alpha)}{K_\alpha h_x^\beta}$, $\mu_2 = \frac{K_\beta \tau^\alpha \Gamma(2-\alpha)}{K_\alpha h_y^\beta}$, $\mu_3 = \frac{K_\beta \tau^\alpha \Gamma(2-\alpha)}{K_\alpha h_z^\beta}$, and noting that the coefficients μ_0, μ_1, μ_2, $\mu_3 > 0$ for $0 < \alpha \leq 1$ and $1 < \beta \leq 2$.

Remark 2: If we use the implicit method to approximate the nonlinear source term, the numerical method of the ST-FBTE can be written as:

$$m_{i,j,k}^{n+1} + \mu_1 \sum_{p=-N_1+i}^{i} \omega_p m_{i-p,j,k}^{n+1} + \mu_2 \sum_{q=-N_2+j}^{j} \omega_q m_{i,j-q,k}^{n+1} + \mu_3 \sum_{r=-N_3+k}^{k} \omega_r m_{i,j,k-r}^{n+1} = \sum_{l=0}^{n-1} (b_l - b_{l+1}) m_{i,j,k}^{n-l} + b_n m_{i,j,k}^{0} + \mu_0 f_{i,j,k}^{n+1}, \tag{22}$$

namely, replace $f_{i,j,k}^{n}$ in (21) with $f_{i,j,k}^{n+1}$. This numerical method is stable and convergent when the nonlinear source term $f(M, \mathbf{r}, t)$ satisfies the local Lipschitz condition (13) (see [21]).

Lemma 1. The coefficients b_l $(l = 0, 1, 2, \cdots)$ satisfy:

(1) $b_0 = 1$, $b_l > 0$ for $l = 1, 2, \cdots$;

(2) $b_l > b_{l+1}$ for $l = 0, 1, 2, \cdots$.

Proof: See [11].

Lemma 2. The coefficients ω_p $(p \in \mathbb{N})$ satisfy:
(1) $\omega_0 \geq 0$, $\omega_{-k} = \omega_k \leq 0$ *for all* $|k| \geq 1$;
(2) $\sum\limits_{p=-\infty}^{\infty} \omega_p = 0$;
(3) For any positive integer n, m with $n < m$, we have $\sum\limits_{p=-m+n}^{n} \omega_p > 0$.

Proof: See [3,16].

4 Solvability of the implicit numerical method

We let $M^{n+1} = [m_{1,1,1}^{n+1}, m_{2,1,1}^{n+1}, \cdots, m_{N_1-1,N_2-1,N_3-1}^{n+1}]^T$, $N^* = (N_1-1)(N_2-1)(N_3-1)$, and $M^0 = [g_{1,1,1}, g_{2,1,1}, \cdots, g_{N_1-1,N_2-1,N_3-1}]^T$, respectively, then the implicit difference approximation (21) can be written in matrix form as

$$(I + A)M^{n+1} = \sum_{l=0}^{n-1} (b_l - b_{l+1}) M^{n-l} + b_n M^0 + \mu_0 F^n, \tag{23}$$

where $F^n = [f_{1,1,1}^n, f_{2,1,1}^n, \cdots, f_{N_1-1,N_2-1,N_3-1}^n]^T$, $I \in \mathbb{R}^{N^* \times N^*}$ is the identity matrix. $A = [a_{sv}] \in \mathbb{R}^{N^* \times N^*}$ is a coefficient matrix. If $s = v$ for $s = 1, 2, \cdots, N^*$, then we obtain

$$a_{ss} = \omega_0(\mu_1 + \mu_2 + \mu_3). \tag{24}$$

In addition, let $s^* = (k-1)(N_3-1) + (j-1)(N_2-1) + i$, then we have

$$\begin{aligned} &\sum_{r=1}^{N_3-1} \sum_{q=1}^{N_2-1} \sum_{p=1}^{N_1-1} a_{s^*,(r-1)(N_3-1)+(q-1)(N_2-1)+p} - a_{s^*,s^*} \\ &= \mu_1 \sum_{p=-N_1+i, p\neq 0}^{i} \omega_p + \mu_2 \sum_{q=-N_2+j, q\neq 0}^{j} \omega_q + \mu_3 \sum_{r=-N_3+k, r\neq 0}^{k} \omega_r, \end{aligned} \tag{25}$$

for $i = 1, 2, \cdots, N_1 - 1, j = 1, 2, \cdots, N_2 - 1, k = 1, 2, \cdots, N_3 - 1$.

Theorem 1. The difference equation defined by (23) is uniquely solvable.

Proof: Let λ be the eigenvalue of the matrix A. Then by the Gerschgorin's circle theorem [19] and Lemma 2, we have

$$\begin{aligned} &|\lambda - \omega_0(\mu_1 + \mu_2 + \mu_3)| \leq r_i \\ &= \mu_1 \sum_{p=-N_1+i, p\neq 0}^{i} |\omega_p| + \mu_2 \sum_{q=-N_2+j, q\neq 0}^{j} |\omega_q| + \mu_3 \sum_{r=-N_3+k, r\neq 0}^{k} |\omega_r| \\ &< \omega_0(\mu_1 + \mu_2 + \mu_3), \end{aligned} \tag{26}$$

where $\sum\limits_{p=-\infty, p\neq 0}^{\infty} |\omega_p| = \omega_0$, $\sum\limits_{q=-\infty, q\neq 0}^{\infty} |\omega_q| = \omega_0$ and $\sum\limits_{r=-\infty, r\neq 0}^{\infty} |\omega_r| = \omega_0$, that is, we have

$$0 < \lambda < 2\omega_0(\mu_1 + \mu_2 + \mu_3). \tag{27}$$

Hence the spectral radius of the matrix $(I + A)$ is greater than one. Therefore, the difference equation defined by (23) is uniquely solvable.

5 Stability of the implicit numerical method

In this section, we prove the stability of the implicit numerical method for the ST-FBTE.

Let $\widetilde{m}^n_{i,j,k}$ be the approximate solution of the implicit numerical method (21), and set $\mathbf{E}^n = [\psi^n_{1,1,1}, \psi^n_{2,1,1}, \cdots, \psi^n_{N_1-1,N_2-1,N_3-1}]^T$, where $\psi^n_{i,j,k} = m^n_{i,j,k} - \widetilde{m}^n_{i,j,k}$, and let $\widetilde{f}^n_{i,j,k}$ be the approximation of $f^n_{i,j,k}$.

Assuming that $\|\mathbf{E}^n\|_\infty = \max\limits_{1\le i\le N_1-1, 1\le j\le N_2-1, 1\le k\le N_3-1} |\psi^n_{i,j,k}|$, then we can obtain the following theorem by mathematical induction.

Theorem 2. The implicit numerical method defined by (21) is unconditionally stable, and there is a positive constant C_1^*, such that

$$\|\mathbf{E}^{n+1}\|_\infty \le C_1^* \|\mathbf{E}^0\|_\infty, \qquad n = 0, 1, 2, \cdots.$$

Proof: From (21), the error $\psi^n_{i,j,k}$ satisfies

$$\begin{aligned}
&\psi^{n+1}_{i,j,k} + \mu_1 \sum_{p=-N_1+i}^{i} \omega_p \psi^{n+1}_{i-p,j,k} + \mu_2 \sum_{q=-N_2+j}^{j} \omega_q \psi^{n+1}_{i,j-q,k} + \mu_3 \sum_{r=-N_3+k}^{k} \omega_r \psi^{n+1}_{i,j,k-r} \\
&= \sum_{m=0}^{n-1} (b_m - b_{m+1}) \psi^{n-m}_{i,j,k} + b_n \psi^0_{i,j,k} + \mu_0 (f^n_{i,j,k} - \widetilde{f}^n_{i,j,k}),
\end{aligned} \tag{28}$$

for $i = 1, 2, \cdots, N_1-1$, $j = 1, 2, \cdots, N_2-1$, $k = 1, 2, \cdots, N_3-1$. Since f satisfies the local Lipschitz condition (13), we have

$$|f^n_{i,j,k} - \widetilde{f}^n_{i,j,k}| \le L_n |\psi^n_{i,j,k}|. \tag{29}$$

When $n = 0$, assume that $\|\mathbf{E}^1\|_\infty = \max\limits_{1\le i\le N_1-1, 1\le j\le N_2-1, 1\le k\le N_3-1} |\psi^1_{i,j,k}| = |\psi^1_{i_*,j_*,k_*}|$. Using Lemma 2, and noting that $\mu_1, \mu_2, \mu_3 > 0$ we have

$$\begin{aligned}
&\|\mathbf{E}^1\|_\infty = |\psi^1_{i_*,j_*,k_*}| \\
&\le |\psi^1_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p |\psi^1_{i_*,j_*,k_*}| + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q |\psi^1_{i_*,j_*,k_*}| \\
&\quad + \mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r |\psi^1_{i_*,j_*,k_*}| \\
&= [1 + \omega_0(\mu_1 + \mu_2 + \mu_3)] |\psi^1_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*, p\neq 0}^{i_*} \omega_p |\psi^1_{i_*,j_*,k_*}| \\
&\quad + \mu_2 \sum_{q=-N_2+j_*, q\neq 0}^{j_*} \omega_q |\psi^1_{i_*,j_*,k_*}| + \mu_3 \sum_{r=-N_3+k_*, r\neq 0}^{k_*} \omega_r |\psi^1_{i_*,j_*,k_*}| \\
&\le [1 + \omega_0(\mu_1 + \mu_2 + \mu_3)] |\psi^1_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*, p\neq 0}^{i_*} \omega_p |\psi^1_{i_*-p,j_*,k_*}|
\end{aligned}$$

$$+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q |\psi^1_{i_*,j_*-q,k_*}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r |\psi^1_{i_*,j_*,k_*-r}|.$$

With the well known inequality $|Z_1| - |Z_2| \leq |Z_1 - Z_2|$, using Lemma 1 we have

$$\begin{aligned}
&\|\mathbf{E}^1\|_\infty = |\psi^1_{i_*,j_*,k_*}| \\
\leq &\Bigg|[1+\omega_0(\mu_1+\mu_2+\mu_3)]\psi^1_{i_*,j_*,k_*} + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p \psi^1_{i_*-p,j_*,k_*} \\
&+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q \psi^1_{i_*,j_*-q,k_*} + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r \psi^1_{i_*,j_*,k_*-r}\Bigg| \\
= &\Bigg|\psi^1_{i_*,j_*,k_*} + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p \psi^1_{i_*-p,j_*,k_*} + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q \psi^1_{i_*,j_*-q,k_*} \\
&+\mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r \psi^1_{i_*,j_*,k_*-r}\Bigg| \\
= &|b_0 \psi^0_{i_*,j_*,k_*} + \mu_0 (f^0_{i,j,k} - \widetilde{f}^0_{i,j,k})|.
\end{aligned}$$

Using local Lipschitz condition (29), we have

$$\begin{aligned}
\|\mathbf{E}^1\|_\infty &\leq |\psi^0_{i_*,j_*,k_*}| + \mu_0 L_0 |\psi^0_{i_*,j_*,k_*}| \leq |\psi^0_{i_*,j_*,k_*}| + \mu_0 L_{\max} |\psi^0_{i_*,j_*,k_*}| \\
&= (1+\mu_0 L_{\max})|\psi^0_{i_*,j_*,k_*}| = (1+\mu_0 L_{\max})\|\mathbf{E}^0\|_\infty.
\end{aligned}$$

Let $\xi = 1 + \mu_0 L_{\max}$, thus, $\|\mathbf{E}^1\|_\infty \leq \xi \|\mathbf{E}^0\|_\infty$.

Now, we suppose that $\|\mathbf{E}^m\|_\infty \leq \xi \|\mathbf{E}^0\|_\infty, m = 1, 2, \cdots, n$. Assuming $\|\mathbf{E}^{n+1}\|_\infty = \max_{1\leq i\leq N_1-1, 1\leq j\leq N_2-1, 1\leq k\leq N_3-1} |\psi^{n+1}_{i,j,k}| = |\psi^{n+1}_{i_*,j_*,k_*}|$, and using Lemma 2 again, we can obtain

$$\begin{aligned}
&\|\mathbf{E}^{n+1}\|_\infty = |\psi^{n+1}_{i_*,j_*,k_*}| \\
\leq &|\psi^{n+1}_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p |\psi^{n+1}_{i_*,j_*,k_*}| + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q |\psi^{n+1}_{i_*,j_*,k_*}| \\
&+\mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r |\psi^{n+1}_{i_*,j_*,k_*}| \\
= &[1+\omega_0(\mu_1+\mu_2+\mu_3)]|\psi^{n+1}_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p |\psi^{n+1}_{i_*,j_*,k_*}| \\
&+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q |\psi^{n+1}_{i_*,j_*,k_*}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r |\psi^{n+1}_{i_*,j_*,k_*}|
\end{aligned}$$

$$\leq [1+\omega_0(\mu_1+\mu_2+\mu_3)]|\psi^{n+1}_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p |\psi^{n+1}_{i_*-p,j_*,k_*}|$$
$$+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q |\psi^{n+1}_{i_*,j_*-q,k_*}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r |\psi^{n+1}_{i_*,j_*,k_*-r}|.$$

Using inequality $|Z_1|-|Z_2| \leq |Z_1-Z_2|$ and Lemma 1 again, we have

$$\begin{aligned}
&\|\mathbf{E}^{n+1}\|_\infty \\
&\leq \Bigg| [1+\omega_0(\mu_1+\mu_2+\mu_3)]\psi^{n+1}_{i_*,j_*,k_*} + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p \psi^{n+1}_{i_*-p,j_*,k_*} \\
&\quad +\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q \psi^{n+1}_{i_*,j_*-q,k_*} + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r \psi^{n+1}_{i_*,j_*,k_*-r} \Bigg| \\
&= \Bigg| \psi^{n+1}_{i_*,j_*,k_*} + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p \psi^{n+1}_{i_*-p,j_*,k_*} + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q \psi^{n+1}_{i_*,j_*-q,k_*} \\
&\quad +\mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r \psi^{n+1}_{i_*,j_*,k_*-r} \Bigg| \\
&= \left| \sum_{m=0}^{n-1} (b_m - b_{m+1}) \psi^{n-m}_{i_*,j_*,k_*} + b_n \psi^0_{i_*,j_*,k_*} + \mu_0 (f^n_{i,j,k} - \widetilde{f}^n_{i,j,k}) \right|.
\end{aligned}$$

Using local Lipschitz condition (29) again, we have

$$\begin{aligned}
\|\mathbf{E}^{n+1}\|_\infty &\leq \sum_{m=0}^{n-1} (b_m - b_{m+1}) \|\mathbf{E}^{n-m}\|_\infty + b_n \|\mathbf{E}^0\|_\infty + \mu_0 L_n |\psi^n_{i_*,j_*,k_*}| \\
&\leq \xi \sum_{m=0}^{n-1} (b_m - b_{m+1}) \|\mathbf{E}^0\|_\infty + b_n \|\mathbf{E}^0\|_\infty + \mu_0 L_{\max} \|\mathbf{E}^n\|_\infty \\
&\leq (b_n + b_0\xi - b_n\xi) \|\mathbf{E}^0\|_\infty + \xi \mu_0 L_{\max} \|\mathbf{E}^0\|_\infty \\
&= (\xi^2 - b_n \mu_0 L_{\max}) \|\mathbf{E}^0\|_\infty.
\end{aligned}$$

From Lemma 1, we know that $b_0 = 1$ and $b_n \to 0$ as $n \to \infty$. Also, note that $\xi = 1 + \mu_0 L_{\max}$, then it is easy to know that $\xi^2 - b_n\mu_0 L_{\max} > 0$. Hence, let $C_1^* = \xi^2 - b_n \mu_0 L_{\max}$, we have

$$\|\mathbf{E}^{n+1}\|_\infty \leq C_1^* \|\mathbf{E}^0\|_\infty. \tag{30}$$

Hence the implicit numerical method defined by (21) is unconditionally stable.

Remark 3: If we use an implicit method to approximate the nonlinear source term, as shown in Remark 2, we can prove that the numerical method defined in (22) is stable when $1 - \mu_0 L_{\max} > 0$, which is independent of the spatial step. In fact, when the time step is small, the condition $1-\mu_0 L_{\max}>0$ is generally satisfied.

6 Convergence of the implicit numerical method

In this section, we prove the convergence of the implicit numerical method for the ST-FBTE.

Setting $\theta_{i,j,k}^n = m(x_i,y_j,z_k,t_n) - m_{i,j,k}^n$, and denoting

$$\mathbf{R}^n = [\theta_{1,1,1}^n, \theta_{2,1,1}^n, \cdots, \theta_{N_1-1,N_2-1,N_3-1}^n]^T,$$

where $\mathbf{R}^0 = \mathbf{0}$. Note that $\mathbf{R}^n$ and $\mathbf{0}$ are $((N_1-1)\times(N_2-1)\times(N_3-1))$ vectors, respectively.

From (10)-(21), the error $\theta_{i,j,k}^n$ satisfies

$$\begin{aligned}
&\theta_{i,j,k}^{n+1} + \mu_1 \sum_{p=-N_1+i}^{i} \omega_p \theta_{i-p,j,k}^{n+1} + \mu_2 \sum_{q=-N_2+j}^{j} \omega_q \theta_{i,j-q,k}^{n+1} + \mu_3 \sum_{r=-N_3+k}^{k} \omega_r \theta_{i,j,k-r}^{n+1} \\
&= \sum_{m=0}^{n-1} (b_m - b_{m+1}) \theta_{i,j,k}^{n-m} + \mu_0 (f(M(x_i,y_j,z_k,t_n),x_i,y_j,z_k,t_n) - f_{i,j,k}^n) \\
&\quad + C_1 \tau^\alpha (\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2), \qquad (31)
\end{aligned}$$

for $i=1,2,\cdots,N_1-1, j=1,2,\cdots,N_2-1, k=1,2,\cdots,N_3-1$.

Since f satisfies the local Lipschitz condition (13), we have

$$|f(M(x_i,y_j,z_k,t_n),x_i,y_j,z_k,t_n) - f_{i,j,k}^n| \le L_n |\theta_{i,j,k}^n|. \qquad (32)$$

Assuming $\|\mathbf{R}^{n+1}\|_\infty = \max\limits_{1\le i\le N_1-1, 1\le j\le N_2-1, 1\le k\le N_3-1} |\theta_{i,j,k}^{n+1}|$, then we can obtain the following theorem by mathematical induction.

Theorem 3. The implicit difference approximation defined by (21) is convergent, and there is a positive constant C^*, such that

$$\|\mathbf{R}^{n+1}\|_\infty \le C^*(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2), \quad n=0,1,2,\cdots. \qquad (33)$$

Proof: When $n=0$, assume that $\|\mathbf{R}^1\|_\infty = \max\limits_{1\le i\le N_1-1, 1\le j\le N_2-1, 1\le k\le N_3-1} |\theta_{i,j,k}^1| = |\theta_{i_*,j_*,k_*}^1|$. Similarly, using Lemma 2, and noting that $\mu_1,\mu_2,\mu_3>0$, we have

$$\begin{aligned}
&\|\mathbf{R}^1\|_\infty = |\theta_{i_*,j_*,k_*}^1| \\
&\le |\theta_{i_*,j_*,k_*}^1| + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p |\theta_{i_*,j_*,k_*}^1| + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q |\theta_{i_*,j_*,k_*}^1| \\
&\quad + \mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r |\theta_{i_*,j_*,k_*}^1|
\end{aligned}$$

$$
\begin{aligned}
&= [1+\omega_0(\mu_1+\mu_2+\mu_3)]|\theta^1_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p|\theta^1_{i_*,j_*,k_*}| \\
&\quad +\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q|\theta^1_{i_*,j_*,k_*}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r|\theta^1_{i_*,j_*,k_*}| \\
&\leq [1+\omega_0(\mu_1+\mu_2+\mu_3)]|\theta^1_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p|\theta^1_{i_*-p,j_*,k_*}| \\
&\quad +\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q|\theta^1_{i_*,j_*-q,k_*}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r|\theta^1_{i_*,j_*,k_*-r}|.
\end{aligned}
$$

Let $\mathbf{V} = C_1\tau^\alpha(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2)$, using inequality $|Z_1| - |Z_2| \leq |Z_1 - Z_2|$, Lemma 1 and local Lipschitz condition (32), we have

$$
\begin{aligned}
\|\mathbf{R}^1\|_\infty &\leq \Bigg| [1+\omega_0(\mu_1+\mu_2+\mu_3)]\theta^1_{i_*,j_*,k_*} + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p\theta^1_{i_*-p,j_*,k_*} \\
&\quad +\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q\theta^1_{i_*,j_*-q,k_*} + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r\theta^1_{i_*,j_*,k_*-r} \Bigg| \\
&= \Bigg| \theta^1_{i_*,j_*,k_*} + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p\theta^1_{i_*-p,j_*,k_*} + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q\theta^1_{i_*,j_*-q,k_*} \\
&\quad +\mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r\theta^1_{i_*,j_*,k_*-r} \Bigg| \\
&= |\mu_0(f(M(x_{i_*},y_{j_*},z_{k_*},t_0),x_{i_*},y_{j_*},z_{k_*},t_0) - f^0_{i_*,j_*,k_*}) + \mathbf{V}| \\
&\leq |\mu_0 L_0\theta^0_{i_*,j_*,k_*} + \mathbf{V}| = b_0^{-1}\mathbf{V}.
\end{aligned}
$$

Now, we suppose that $\|\mathbf{R}^m\|_\infty \leq b_{m-1}^{-1}\mathbf{V}$, $m = 1, 2, \cdots, n$. Assuming $\|\mathbf{R}^{n+1}\|_\infty = \max_{1\leq i\leq N_1-1, 1\leq j\leq N_2-1, 1\leq k\leq N_3-1} |\theta^{n+1}_{i,j,k}| = |\theta^{n+1}_{i_*,j_*,k_*}|$, and using Lemma 2 again we have

$$
\begin{aligned}
&\|\mathbf{R}^{n+1}\|_\infty = |\theta^{n+1}_{i_*,j_*,k_*}| \\
&\leq |\theta^{n+1}_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p|\theta^{n+1}_{i_*,j_*,k_*}| + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q|\theta^{n+1}_{i_*,j_*,k_*}| \\
&\quad +\mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r|\theta^{n+1}_{i_*,j_*,k_*}| \\
&= [1+\omega_0(\mu_1+\mu_2+\mu_3)]|\theta^{n+1}_{i_*,j_*,k_*}| + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p|\theta^{n+1}_{i_*,j_*,k_*}|
\end{aligned}
$$

$$
\begin{aligned}
&+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q |\theta_{i_*,j_*,k_*}^{n+1}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r |\theta_{i_*,j_*,k_*}^{n+1}| \\
&\leq [1+\omega_0(\mu_1+\mu_2+\mu_3)]|\theta_{i_*,j_*,k_*}^{n+1}| + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p |\theta_{i_*-p,j_*,k_*}^{n+1}| \\
&+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q |\theta_{i_*,j_*-q,k_*}^{n+1}| + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r |\theta_{i_*,j_*,k_*-r}^{n+1}|.
\end{aligned}
$$

Using inequality $|Z_1|-|Z_2| \leq |Z_1-Z_2|$ and Lemma 1 again, we have

$$
\begin{aligned}
&\|\mathbf{R}^{n+1}\|_\infty \\
&\leq \Bigg| [1+\omega_0(\mu_1+\mu_2+\mu_3)]\theta_{i_*,j_*,k_*}^{n+1} + \mu_1 \sum_{p=-N_1+i_*,p\neq 0}^{i_*} \omega_p \theta_{i_*-p,j_*,k_*}^{n+1} \\
&+\mu_2 \sum_{q=-N_2+j_*,q\neq 0}^{j_*} \omega_q \theta_{i_*,j_*-q,k_*}^{n+1} + \mu_3 \sum_{r=-N_3+k_*,r\neq 0}^{k_*} \omega_r \theta_{i_*,j_*,k_*-r}^{n+1} \Bigg| \\
&= \Bigg| \theta_{i_*,j_*,k_*}^{n+1} + \mu_1 \sum_{p=-N_1+i_*}^{i_*} \omega_p \theta_{i_*-p,j_*,k_*}^{n+1} + \mu_2 \sum_{q=-N_2+j_*}^{j_*} \omega_q \theta_{i_*,j_*-q,k_*}^{n+1} \\
&+\mu_3 \sum_{r=-N_3+k_*}^{k_*} \omega_r \theta_{i_*,j_*,k_*-r}^{n+1} \Bigg| \\
&= \Bigg| \sum_{m=0}^{n-1} (b_m - b_{m+1}) \theta_{i_*,j_*,k_*}^{n-m} + \mu_0 (f(M(x_{i_*}, y_{j_*}, z_{k_*}, t_n), x_{i_*}, y_{j_*}, z_{k_*}, t_n) \\
&-f_{i_*,j_*,k_*}^n) + \mathbf{V} \Bigg|.
\end{aligned}
$$

Using local Lipschitz condition (32) again, we have

$$
\begin{aligned}
\|\mathbf{R}^{n+1}\|_\infty &\leq \left| \sum_{m=0}^{n-1} (b_m - b_{m+1}) \theta_{i_*,j_*,k_*}^{n-m} + \mu_0 L_n \theta_{i_*,j_*,k_*}^n + \mathbf{V} \right| \\
&\leq \sum_{m=0}^{n-1} (b_m - b_{m+1}) b_{n-m-1}^{-1} \mathbf{V} + \mu_0 L_{\max} b_{n-1}^{-1} \mathbf{V} + \mathbf{V} \\
&\leq \sum_{m=0}^{n-1} (b_m - b_{m+1}) b_n^{-1} \mathbf{V} + \mu_0 L_{\max} b_n^{-1} \mathbf{V} + \mathbf{V} \\
&= b_n^{-1} (b_0 - b_n + \mu_0 L_{\max} + b_n) \mathbf{V} \\
&= b_n^{-1} (b_0 + \mu_0 L_{\max}) \mathbf{V} \\
&= \xi b_n^{-1} \mathbf{V}.
\end{aligned}
$$

Noting that $\mathbf{V} = C_1\tau^{\alpha}(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2)$, and

$$\lim_{n\to\infty}\frac{b_n^{-1}}{n^{\alpha}} = \lim_{n\to\infty}\frac{n^{-\alpha}}{(n+1)^{1-\alpha} - n^{1-\alpha}} = \frac{1}{1-\alpha},$$

therefore there exists a positive constant C_2, such that

$$\|\mathbf{R}^{n+1}\|_{\infty} \le \xi C_1 C_2 n^{\alpha}\tau^{\alpha}(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2).$$

Finally, noting that $n\tau \le T$ is finite, so there exists a positive constant C^*, such that $\|\mathbf{R}^{n+1}\|_{\infty} \le C^*(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2)$ for $n = 0, 1, 2, \cdots$.

Hence, the implicit numerical method defined by (21) is convergent.

Remark 4: If we use an implicit method to approximate the nonlinear source term, as shown in Remark 2, we can prove that the numerical method defined in (22) is convergent when $1 - \mu_0 L_{\max} > 0$, which is independent of the spatial step. In fact, when the time step is small, the condition $1 - \mu_0 L_{\max} > 0$ is generally satisfied.

7 Numerical results

Due to the computational overheads necessary to perform the simulations for the space and time fractional Bloch-Torrey equation in three dimensions, we present here a preliminary study based on a two-dimensional example to confirm our theoretical analysis.

In example 1, we use the same example in [24], where the source term depends only on space and time, for comparison to show that our new implicit numerical method can obtain second order space accuracy, which is $O(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2)$.

Example 1.

The following time and space Riesz fractional diffusion equation with initial and zero Dirichlet boundary conditions on a finite domain is considered (See [24]):

$$K_{\alpha}\ {}_0^C D_t^{\alpha} M(\mathbf{r}, t) = K_{\beta}(\frac{\partial^{\beta}}{\partial|x|^{\beta}} + \frac{\partial^{\beta}}{\partial|y|^{\beta}})M(\mathbf{r}, t) + f(\mathbf{r}, t), \quad (34)$$

$$M(\mathbf{r}, 0) = 0, \quad (35)$$

$$M(\mathbf{r}, t)|_{\bar{\Omega}} = 0, \quad (36)$$

where

$$\begin{aligned} f(\mathbf{r}, t) = \frac{K_{\beta}t^{\alpha+\beta}}{2cos(\beta\pi/2)}((&\frac{2}{\Gamma(3-\beta)}[x^{2-\beta} + (1-x)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)}[x^{3-\beta} \\ &+(1-x)^{3-\beta}] + \frac{24}{\Gamma(5-\beta)}[x^{4-\beta} + (1-x)^{4-\beta}])y^2(1-y)^2 \\ &+(\frac{2}{\Gamma(3-\beta)}[y^{2-\beta} + (1-y)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)}[y^{3-\beta} + (1-y)^{3-\beta}] \end{aligned}$$

$$+\frac{24}{\Gamma(5-\beta)}[y^{4-\beta}+(1-y)^{4-\beta}])x^2(1-x)^2)$$
$$+\frac{K_\alpha\Gamma(\alpha+\beta+1)}{\Gamma(\beta+1)}t^\beta x^2(1-x)^2)y^2(1-y)^2, \quad (37)$$

and $0 < \alpha \le 1$, $1 < \beta \le 2$, $t > 0$, $\mathbf{r} = (x, y) \in \Omega$, Ω is the finite rectangular region $[0, 1] \times [0, 1]$, and $\bar{\Omega}$ is $\mathcal{R}^2 - \Omega$.

The exact solution of this problem is $M(\mathbf{r}, t) = t^{\alpha+\beta}x^2(1-x)^2y^2(1-y)^2$, which can be verified by substituting directly into (34).

When $K_\alpha = 1.0, K_\beta = 0.5, \alpha = 0.8$, and $\beta = 1.8$, Table 1 lists the maximum absolute error between the exact solution and the numerical solutions obtained by the implicit numerical method, with spatial and temporal steps $\tau^{\frac{2-\alpha}{2}} \approx h_x = h_y = 1/4, 1/8, 1/16, 1/32$ at time $t = 1.0$

Table 1 Comparison of maximum error for the implicit numerical method at time $t = 1.0$

$\tau^{\frac{2-\alpha}{2}} \approx h_x = h_y$	Maximum error	Error rate
$\frac{1}{4}$	0.000591593	-
$\frac{1}{8}$	0.000141157	4.20≈ 4
$\frac{1}{16}$	0.0000342583	4.12≈ 4
$\frac{1}{32}$	0.00000835079	4.10≈ 4

From Table 1, it can be seen that the

$$Error\ rate = \frac{error(h)^2}{error(\frac{1}{2}h)^2} \approx 4.$$

This is in good agreement with our theoretical analysis, namely the convergence order of the implicit numerical method for this problem is $O(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2)$.

We now exhibit in example 2 the solution profiles of the time and space Riesz fractional diffusion equation with a nonlinear source term.

Example 2.

Nonlinear time and space Riesz fractional diffusion equation with initial and zero Dirichlet boundary conditions on a finite domain:

$$K_\alpha\, {}_0^C D_t^\alpha M(\mathbf{r}, t) = K_\beta(\frac{\partial^\beta}{\partial|x|^\beta} + \frac{\partial^\beta}{\partial|y|^\beta})M(\mathbf{r}, t) + f(M, \mathbf{r}, t), \quad (38)$$
$$M(\mathbf{r}, 0) = \min\{1.0, 10e^{-x^2-y^2}\}, \quad (39)$$
$$M(\mathbf{r}, t)|_{\bar{\Omega}} = 0, \quad (40)$$

where the nonlinear source term is Fisher's growth equation $f(M, \mathbf{r}, t) = 0.25M(\mathbf{r}, t)[1 - M(\mathbf{r}, t)]$, and $0 < \alpha \le 1$, $1 < \beta \le 2$, $t > 0$, $\mathbf{r} = (x, y) \in \Omega$, Ω is the finite rectangular region $[0, 1] \times [0, 1]$, and $\bar{\Omega}$ is $\mathcal{R}^2 - \Omega$.

The solution profiles of (38) by the implicit numerical method, with spatial and temporal steps $h_x = h_y = 1/32$, $\tau = 1/322$ at time $t = 32/322$ with

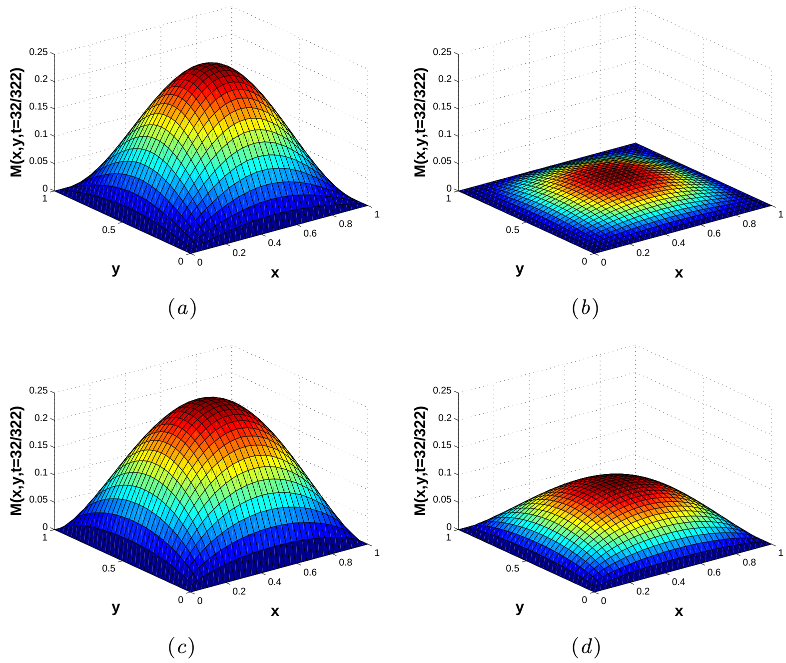

Fig. 1 A plot of numerical solutions of ST-FBTE using the implicit numerical method (INM) with spatial and temporal steps $h_x = h_y = 1/32$, $\tau = 1/322$ at time $t = 32/322$ with $K_\alpha = 1.0, t_{final} = 1.0$ for different α, β and K_β. (a) $\alpha = 1.0, \beta = 2.0, K_\beta = 1.0$. (b) $\alpha = 1.0, \beta = 2.0, K_\beta = 2.0$. (c) $\alpha = 0.8, \beta = 1.8, K_\beta = 1.0$. (d) $\alpha = 0.8, \beta = 1.8, K_\beta = 2.0$.

$K_\alpha = 1.0, t_{final} = 1.0$ for different α, β and K_β are listed in Figure 1. From Figure 1, it can be seen that the coefficient K_β impacts on the solution profiles of (38), whereby a larger value of K_β produces more diffuse profiles.

In Figure 2, we illustrate the effect of the fractional order in space for this problem, with spatial and temporal steps $h_x = h_y = 1/32$, $\tau = 1/322$ at time $t = 32/322$ with $K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 1.0$ for β fixed at 2 and α varying. From Figure 2, it can be seen that as α is decreased the diffusion profiles becomes more pronounced.

In Figure 3, we illustrate the effect of the fractional order in time for this problem, with spatial and temporal steps $h_x = h_y = 1/32$, $\tau = 1/322$ at time $t = 32/322$ with $K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 1.0$ for α fixed at 1 and β varying. From Figure 3, it can be seen that as β is reduced the diffusion becomes more pronounced.

8 Conclusions

In this paper, a new effective implicit numerical method for solving the fractional Bloch-Torrey equation in three-dimensions with a nonlinear source term

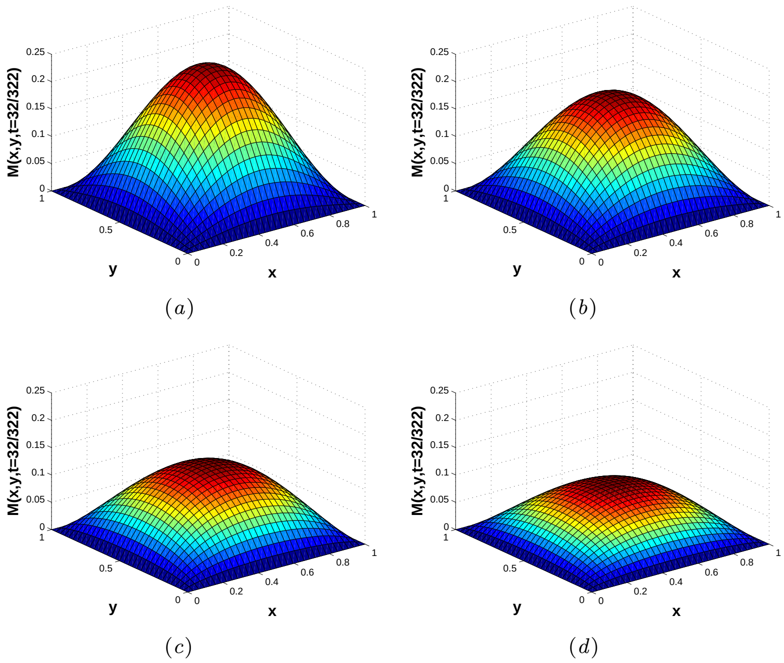

Fig. 2 A plot of numerical solutions of ST-FBTE using the implicit numerical method (INM) with spatial and temporal steps $h_x = h_y = 1/32$, $\tau = 1/322$ at time $t = 32/322$ with $K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 1.0$ for β fixed at 2. (a) $\alpha = 1.0$. (b) $\alpha = 0.9$. (c) $\alpha = 0.5$. (d) $\alpha = 0.2$.

has been derived. We prove that the implicit numerical method is uniquely solvable, unconditionally stable and convergent. In addition, compared with first order spatial accuracy of convergence in [24], and the two-dimensional model with a linear source term in [25], our new implicit numerical method can obtain second order space accuracy, which is $O(\tau^{2-\alpha} + \tau + h_x^2 + h_y^2 + h_z^2)$.

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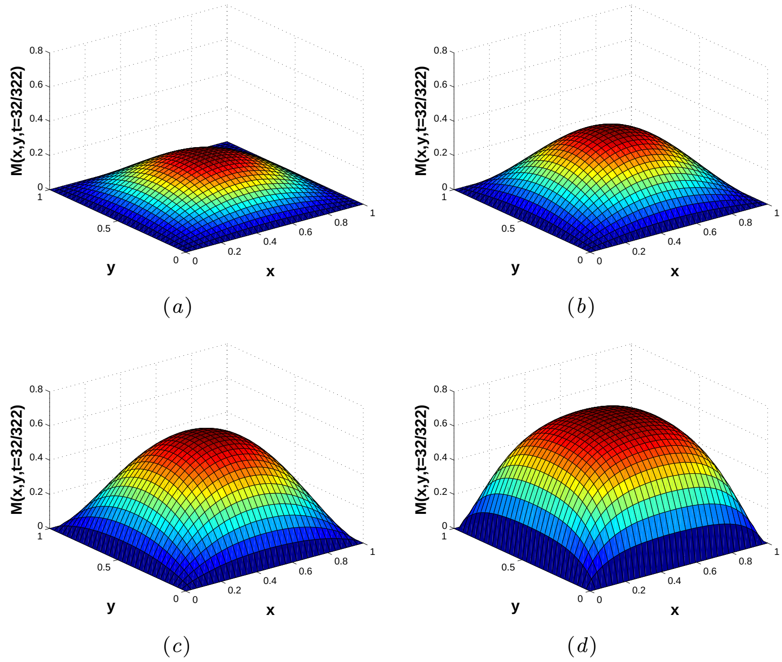

Fig. 3 A plot of numerical solutions of ST-FBTE using the implicit numerical method (INM) with spatial and temporal steps $h_x = h_y = 1/32$, $\tau = 1/322$ at time $t = 32/322$ with $K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 1.0$ for α fixed at 1. (a) $\beta = 2.0$. (b) $\beta = 1.8$. (c) $\beta = 1.5$. (d) $\beta = 1.2$.

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