A computationally effective alternating direction method for the space and time fractional Bloch-Torrey equation in 3-D

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Abstract

The space and time fractional Bloch-Torrey equation (ST-FBTE) has been used to study anomalous diffusion in the human brain. Numerical methods for solving ST-FBTE in three-dimensions are computationally demanding. In this paper, we propose a computationally effective fractional alternating direction method (FADM) to overcome this problem. We consider ST-FBTE on a finite domain where the time and space derivatives are replaced by the Caputo-Djrbashian and the sequential Riesz fractional derivatives, respectively. The stability and convergence properties of the FADM are discussed. Finally, some numerical results for ST-FBTE are given to confirm our theoretical findings.

Key words: Fractional Bloch-Torrey Equation, fractional calculus, implicit numerical method, alternating direction method, stability, convergence

1. Introduction

Recently, fractional order calculus has been used to examine the connection between fractional order dynamics and diffusion to solve the Bloch-Torrey equation \cite{1, 2, 3, 4, 5}. It was pointed out that a fractional diffusion model could be successfully applied to analyzing diffusion images of human brain tissues and provide new insights into further investigations of tissue
structures and the microenvironment. Magin et al. [1] proposed a new diffusion model for solving the Bloch-Torrey equation using fractional order calculus with respect to time and space. The space-time fractional Bloch-Torrey equation (ST-FBTE) can be written as the following form:

$$\tau^{\alpha-1} C_0^\alpha M_{xy}(r, t) = \lambda M_{xy}(r, t) + D\mu^{2(\beta-1)} R^\beta M_{xy}(r, t),$$

(1)

where \(\lambda = -i\gamma(r \cdot G(t))\), \(r = (x, y, z)\), \(G(t)\) is the magnetic field gradient, \(\gamma\) and \(D\) are the gyromagnetic ratio and the diffusion coefficient respectively. \(C_0^\alpha\) is the Caputo-Djrbashian time fractional derivative of order \(\alpha\) \((0 < \alpha \leq 1)\) with respect to \(t\), and with the starting point at \(t = 0\) is defined regularized as [6]:

$$C_0^\alpha u(x, t) = \frac{1}{\Gamma(1-\alpha)} \left[ \frac{\partial}{\partial t} \int_0^t \frac{u(x, \tau)}{(t-\tau)^\alpha} d\tau - \frac{u(x, 0)}{t^\alpha} \right].$$

(2)

\(R^\beta = (R_x^\beta + R_y^\beta + R_z^\beta)\) is a sequential Riesz fractional order operator in space [7]; \(M_{xy}(r, t) = M_x(r, t) + iM_y(r, t)\), where \(i = \sqrt{-1}\), comprises the transverse components of the magnetization; and \(\tau^{\alpha-1}\) and \(\mu^{2(\beta-1)}\) are the fractional order time and space constants needed to preserve units, \((0 < \alpha \leq 1, \text{ and } 1 < \beta \leq 2)\). Magin et al. [1] derived analytical solutions with fractional order dynamics in space (i.e., \(\alpha = 1\), \(\beta\) an arbitrary real number, \(1 < \beta \leq 2\)) and time (i.e., \(0 < \alpha < 1\), and \(\beta = 2\)), respectively. Yu et al. [2] derived an analytical solution and an effective implicit numerical method for solving equation (1). They also considered the stability and convergence properties of the implicit numerical method. However, due to the computational overheads necessary to perform the simulations for ST-FBTE in three dimensions, they presented a preliminary study based on a two-dimensional example to confirm their theoretical analysis.

Alternating direction implicit (ADI) schemes have been proposed for the numerical simulations of classic differential equations [8, 9, 10]. The ADI schemes reduce the multidimensional problem into a series of independent one-dimensional problems and are thus computationally efficient.

Since fractional derivatives are nonlocal and have history dependence, fractional problems generally require a large amount of CPU time if traditional implicit schemes based on Gaussian elimination are used. In order to overcome the computational difficulty, a number of authors have applied ADI schemes for solving fractional problems. Meerschaert et al. [11] applied a practical ADI method to solve a class of two-dimensional initial-boundary
value space-fractional partial differential equations with variable coefficients on a finite domain. They proved that the ADI method is unconditionally stable and converges linearly. Chen and Liu [12] used a new technique with a combination of the ADI-Euler method, the unshifted Grünwald formula for the advection term, the right-shifted Grünwald formula for the diffusion term, and Richardson extrapolation to establish an unconditionally stable second order accurate difference method for a two-dimensional fractional advection-dispersion equation. Zhang and Sun [13] used ADI schemes for a two-dimensional time-fractional sub-diffusion equation. They proved the method is unconditionally stable and convergent by the discrete energy method, and showed that the computational complexities and CPU time are reduced greatly. Liu et al. [14] proposed a fractional ADI scheme for three-dimensional non-continued seepage flow in uniform media and a modified Douglas scheme for the continued seepage flow in non-uniform media. They proved that both methods are unconditionally stable and convergent.

In this paper, we construct a fractional alternating direction method (FADM) for the three-dimensional space and time fractional Bloch-Torrey equation (ST-FBTE) with initial and boundary conditions on a finite domain, and prove that the FADM for the ST-FBTE is unconditionally stable and convergent.

The structure of the remainder of this paper is as follows. In Section 2, some mathematical preliminaries are introduced. In Section 3, we propose a fractional alternating direction method for ST-FBTE. The stability and convergence of the FADM are investigated in Sections 4 and 5, respectively. Finally, numerical results for ST-FBTE are given to verify our theoretical results.

2. Preliminary knowledge

In this section, we outline some preliminary knowledge used throughout the remaining sections of this paper. It is assumed throughout this section that $M(x, y, z, t) \in C_{x,y,z,t}^{3,3,3,2}(\Omega)$ for $0 < \alpha \leq 1$ and $1 < \beta \leq 2$, where $t \in [0, T]$ and $\Omega : -\infty \leq x, y, z \leq +\infty$.

Definition 1. Let $M$ be as defined above on an infinite interval $\Omega : -\infty \leq x, y, z \leq +\infty$. The Riesz fractional operator $R^\beta$ is defined as [15]

$$R^\beta_x M(x, y, z, t) = \frac{\partial^\beta M(x, y, z, t)}{\partial |x|^\beta} = -c_\beta (\infty D^\beta_x + x D^\beta_+) M(x, y, z, t), \quad (3)$$
where $c_\beta = \frac{1}{2\cos(\frac{\pi \beta}{2})}$, $\beta \neq 1$,

\[-\infty D_x^\beta M(x, y, z, t) = \frac{1}{\Gamma(2 - \beta)} \frac{\partial^2}{\partial x^2} \int_{-\infty}^{x} \frac{M(\xi, y, z, t) d\xi}{(x - \xi)^{\beta-1}},\]

\[\_x D_{+\infty}^\beta M(x, y, z, t) = \frac{(-1)^2}{\Gamma(2 - \beta)} \frac{\partial^2}{\partial x^2} \int_{x}^{+\infty} \frac{M(\xi, y, z, t) d\xi}{(\xi - x)^{\beta-1}}.\]

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

**Lemma 1.** Suppose that $M(x) \in C^{\beta}(-\infty, \infty)$, the following equality holds

\[\frac{\partial^\beta}{\partial |x|^\beta} M(x) = -\frac{1}{2\cos\frac{\pi \beta}{2}} [-\infty D_x^\beta + \_x D_{+\infty}^\beta] M(x),\] (4)

where $1 < \beta \leq 2$.

**Proof.** See [16, 17].

**Lemma 2.** Suppose that $M(x) \in C^{\beta}[0, L]$, the following equality

\[\frac{\partial^\beta}{\partial |x|^\beta} M(x) = -\frac{1}{2\cos\frac{\pi \beta}{2}} [0 D_x^\beta + \_x D_{L}^\beta] M^*(x),\] (5)

also holds when setting

\[M^*(x) = \begin{cases} M(x), & x \in (0, L), \\ 0, & x \notin (0, L), \end{cases}\]

i.e., $M^*(x) = 0$ on the boundary points and beyond the boundary points.

**Proof.** See [16, 17].

The use of Lemmas 1 and 2 above allows us to define the Riesz fractional operator on a bounded set $\Omega$ with zero Dirichlet boundary conditions.

We present our solution techniques for solving the ST-FBTE in the following steps. Firstly, the ST-FBTE (1) is rewritten in the form:

\[K_\alpha C \int_0^t D_t^\alpha M_{xy}(r, t) = \lambda M_{xy}(r, t) + K_\beta R^\beta M_{xy}(r, t).\] (6)
We equate real and imaginary components to express equation (6) as a coupled system of partial differential equations for the components $M_x$ and $M_y$, namely

$$K_\alpha \frac{C}{0} D_t^\alpha M_x (r, t) = \lambda_G M_y (r, t)$$

$$+ K_\beta \left( \frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta} \right) M_x (r, t),$$

$$K_\alpha \frac{C}{0} D_t^\alpha M_y (r, t) = -\lambda_G M_x (r, t)$$

$$+ K_\beta \left( \frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta} \right) M_y (r, t),$$

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

For convenience, the ST-FBTE (7) and (8) are decoupled (see [18]), which is equivalent to solving a fractional in space and time partial differential equation of the form

$$K_\alpha \frac{C}{0} D_t^\alpha M (r, t) = K_\beta \left( \frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta} \right) M (r, t) + f (r, t),$$

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

3. Fractional alternating direction method

We propose a fractional alternating direction method for the space and time fractional Bloch-Torrey equation (9) with initial and boundary conditions on a finite domain given by

$$M (r, 0) = M_0 (r),$$

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

where $0 < \alpha \leq 1$, $1 < \beta \leq 2$, $0 < t \leq T$, $r = (x, y, z) \in \Omega$, $\Omega$ is the finite rectangular region $[0, L_1] \times [0, L_2] \times [0, L_3]$, $M_0 (r) = M_0 (x, y, z)$ is continuous on $\Omega$, and $\bar{\Omega}$ is $\mathbb{R}^3 - \Omega$.

Suppose that the continuous problem (9)-(11) has a smooth solution $M (x, y, z, t) \in C^{3,3,3,2}_{x,y,z,t} (\Omega)$. 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. At a point $(x_i, y_j, z_k)$ at the moment of time $t_n$ for $i, j, k \in \mathcal{N}$ and $n \in \mathcal{N}$, we denote the exact and numerical solutions $M (r, t)$ as $u (x_i, y_j, z_k, t_n)$ and $u^n_{i,j,k}$, respectively.
Firstly, adopting the scheme in [19], we discretize the Caputo-Djrbashian time fractional derivative of $u(x_i, y_j, z_k, t_{n+1})$ as

$$\frac{C_0^\alpha}{\Gamma(2-\alpha)} D_t^{\alpha} u(x_i, y_j, z_k, t) |_{t=t_{n+1}} = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{l=0}^{n} b_l[u(x_i, y_j, z_k, t_{n+1-1}) - u(x_i, y_j, z_k, t_{n-1})] + O(\tau^{2-\alpha}),$$

(12)

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

Using the relationship between the Riemann-Liouville derivative and the Grünwald-Letnikov scheme, we discretize the Riesz fractional derivative by the shifted Grünwald-Letnikov scheme [16]

$$0 \alpha^D \beta u(x, y_j, z_k, t_{n+1}) |_{x=x_i} = \frac{1}{h_x} \sum_{p=0}^{i+1} \omega_p u(x_{i-p+1}, y, z, t_{n+1}) + O(h_x),$$

(13)

$$x \alpha^D \beta L_1 u(x, y_j, z_k, t_{n+1}) |_{x=x_i} = \frac{1}{h_x} \sum_{p=0}^{N_1-i+1} \omega_p u(x_{i+p-1}, y, z, t_{n+1}) + O(h_x),$$

(14)

where the coefficients are defined by

$$\omega_0 = 1, \quad \omega_p = (-1)^p \frac{\beta(\beta - 1) \cdots (\beta - p + 1)}{p!}, \quad p = 1, 2, \cdots, N_1.$$  (15)

Similar results hold for the fractional $y$ and $z$ derivatives.

Thus, we can derive the implicit numerical scheme:

$$\frac{K_\alpha \tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{l=0}^{n} b_l[u_{i,j,k}^{n+1-1} - u_{i,j,k}^{n-1}] - c_\beta K_\beta \left[ \frac{1}{h_x} \sum_{p=0}^{i+1} \omega_p u_{i-p+1,i,j,k}^{n+1} \right]$$

$$+ \sum_{p=0}^{N_1-i+1} \omega_p u_{i+p-1,i,j,k}^{n+1} + \frac{1}{h_y} \left( \sum_{q=0}^{j+1} \omega_q u_{i,j-q+1,k}^{n+1} + \sum_{q=0}^{N_2-j+1} \omega_q u_{i,j+q-1,k}^{n+1} \right)$$

$$+ \frac{1}{h_z} \left( \sum_{r=0}^{k+1} \omega_r u_{i,j,k-r+1}^{n+1} + \sum_{r=0}^{N_3-k+1} \omega_r u_{i,j,k+r-1}^{n+1} \right) + f_{i,j,k}^{n+1}.$$  (16)
Rearranging (16), we then have the following implicit difference approximation:

\[
\begin{align*}
& u_{n+1}^{i,j,k} + \mu_1 \sum_{p=0}^{i+1} \omega_p u_{n+1}^{i-p+1,j,k} + \mu_2 \sum_{q=0}^{j+1} \omega_q u_{n+1}^{i,j-q+1,k} \\
& + \sum_{q=0}^{N_1-j+1} \omega_q u_{n+1}^{i,j+q-1,k} + \mu_3 \left( \sum_{r=0}^{k+1} \omega_r u_{n+1}^{i,j,k-r+1} + \sum_{r=0}^{N_2-k+1} \omega_r u_{n+1}^{i,j,k+r-1} \right) \\
& = \sum_{l=0}^{n-1} \left( b_l - b_{l+1} \right) u_{n+1}^{i-j,k} + b_n u_{n+1}^{0,j,k} + \mu_0 f_{n+1}^{i,j,k},
\end{align*}
\]

\[i = 1, 2, \cdots, N_1 - 1, j = 1, 2, \cdots, N_2 - 1, k = 1, 2, \cdots, N_3 - 1,\]

with

\[
\begin{align*}
& u_{0,j,k}^0 = g_{i,j,k} = g(x_i, y_j, z_k), \\
& u_{0,j,k}^{n+1} = u_{N_1,j,k}^{n+1} = u_{i,0,k}^{n+1} = u_{i,j,0}^{n+1} = u_{i,j,N_3}^{n+1} = 0, \\
& (i = 0, 1, \cdots, N_1, j = 0, 1, \cdots, N_2, k = 0, 1, \cdots, N_3)
\end{align*}
\]

where \( \mu_0 = \frac{r^\alpha \Gamma(2-\alpha)}{K_u}, \mu_1 = \frac{c_3 K_\alpha r^\alpha \Gamma(2-\alpha)}{K_u h_u^2}, \mu_2 = \frac{c_2 K_\alpha r^\alpha \Gamma(2-\alpha)}{K_u h_u^2}, \mu_3 = \frac{c_1 K_\alpha r^\alpha \Gamma(2-\alpha)}{K_u h_u^2}, \)

and noting that coefficients \( \mu_0 > 0, \mu_1, \mu_2, \mu_3 < 0 \) for \( 0 < \alpha \leq 1 \) and \( 1 < \beta \leq 2. \)

**Lemma 3.** 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 [20].

**Lemma 4.** The coefficients \( \omega_p \ (p \in N) \) satisfy:

1. \( \omega_1 = -\beta, \ \omega_p \geq 0 \) \( (p \neq 1); \)
2. \( \sum_{p=0}^{\infty} \omega_p = 0; \)
3. \( \omega_1 < 0, \mu_1, \mu_2, \mu_3 < 0 \) for \( 0 < \alpha \leq 1 \) and \( 1 < \beta \leq 2. \)

**Proof.** See [19, 20].
We consider the following fractional partial differential discrete operator:

\[
\delta_x^\beta u_{i,j,k}^{n+1} = \sum_{p=0}^{i+1} \omega_p u_{i-p+1,j,k}^{n+1} + \sum_{p=0}^{N_i-i+1} \omega_p u_{i+p-1,j,k}^{n+1},
\]

which is an \(O(h_x)\) approximation of the Riesz fractional derivative by the shifted Grünwald-Letnikov scheme (13) and (14) [16]. Similarly, the following fractional partial differential discrete operators:

\[
\begin{align*}
\delta_y^\beta u_{i,j,k}^{n+1} &= \sum_{q=0}^{j+1} \omega_q u_{i,j-q+1,k}^{n+1} + \sum_{q=0}^{N_j-j+1} \omega_q u_{i,j+q-1,k}^{n+1}, \\
\delta_z^\beta u_{i,j,k}^{n+1} &= \sum_{r=0}^{k+1} \omega_r u_{i,j,k-r+1}^{n+1} + \sum_{r=0}^{N_k-k+1} \omega_r u_{i,j,k+r-1}^{n+1},
\end{align*}
\]

are \(O(h_y)\) and \(O(h_z)\) approximation of the Riesz fractional derivatives, respectively.

Thus, the implicit difference scheme (17) may be rearranged in the following form involving \(\delta_x^\beta\), \(\delta_y^\beta\) and \(\delta_z^\beta\):

\[
(1 + \mu_1 \delta_x^\beta + \mu_2 \delta_y^\beta + \mu_3 \delta_z^\beta) u_{i,j,k}^{n+1} = \sum_{l=0}^{n-1} (b_l - b_{l+1}) u_{i,j,k}^{n-l} + b_n u_{i,j,k}^0 + \mu_0 f_{i,j,k}^{n+1}.
\]

The implicit difference scheme (17) for the ST-FBTE has a local truncation error of the form \(O(r^{2-\alpha} + h_x + h_y + h_z)\) and is unconditionally stable (refer to the proof of Theorem 1 in this paper). Unfortunately, (17) provides us with a linear system of equations for calculating the difference solution \(u_{i,j,k}^{n+1}\), that does not have the good property of the coefficient matrix being banded but still has a regular sparse structure in that all the off diagonal blocks are themselves diagonal matrices. However, this can complicate the solution of the corresponding linear system of equations.

Therefore, we adopt the alternating direction implicit method used in [14]. Our aim is to divide the calculation into three steps with reduced calculation. In the first step, we solve the problem in the \(x\)-direction, in the second step, we solve the problem in the \(y\)-direction, finally in the third step we solve the problem in the \(z\)-direction. For example, we introduce an additional negligible term (see Theorem 2)

\[
(\mu_1 \mu_2 \delta_x^\beta \delta_y^\beta + \mu_1 \mu_3 \delta_x^\beta \delta_z^\beta + \mu_2 \mu_3 \delta_y^\beta \delta_z^\beta + \mu_1 \mu_2 \mu_3 \delta_x^\beta \delta_y^\beta \delta_z^\beta) u_{i,j,k}^{n+1}
\]
to the left side of (21) that has no impact on the convergence of the scheme to obtain

\[(1 + \mu_1 \delta_x^3)(1 + \mu_2 \delta_y^3)(1 + \mu_3 \delta_z^3)u_{i,j,k}^{n+1} = \sum_{l=0}^{n-1}(b_l - b_{l+1})u_{i,j,k}^{n-l} + b_n u_{i,j,k}^0 + \mu_0 f_{i,j,k}^{n+1}. \tag{23}\]

Hence, the FADM at time \(t_{n+1}\) is defined as:

\[(1 + \mu_1 \delta_x^3)u_{i,j,k}^{n+1} = \sum_{l=0}^{n-1}(b_l - b_{l+1})u_{i,j,k}^{n-l} + b_n u_{i,j,k}^0 + \mu_0 f_{i,j,k}^{n+1}, \tag{24}\]

\[(1 + \mu_2 \delta_y^3)u_{i,j,k}^{n+2/3} = u_{i,j,k}^{n+1/3}, \tag{25}\]

\[(1 + \mu_3 \delta_z^3)u_{i,j,k}^{n+1} = u_{i,j,k}^{n+2/3}. \tag{26}\]

Together with the boundary values \(u_{0,j,k}^{n+1/3}\) and \(u_{N_1,j,k}^{n+1/3}\) calculated below, the coefficient matrix \(A_{j,k} = (a_{j,k})_{s,t}\) of the linear system (24) can be obtained as follows: for each fixed \((j,k)\),

\[
(a_{j,k})_{s,t} = \begin{cases} 
\mu_1 \omega_{t-s+1}, & t \geq s + 2, s = 1, 2, \ldots, N_1 - 3, \\
\mu_1(\omega_0 + \omega_2), & t = s + 1, s = 1, 2, \ldots, N_1 - 2, \\
1 + 2\mu_1 \omega_1, & t = s + 1, s = 1, 2, \ldots, N_1 - 1, \\
\mu_1(\omega_0 + \omega_2), & t = s - 1, s = 2, \ldots, N_1 - 1, \\
\mu_1 \omega_{s-t+1}, & t \leq s - 2, s = 3, 4, \ldots, N_1 - 1.
\end{cases} \tag{27}\]

The coefficient matrices \(B_{i,k} = (b_{i,k})_{s,t}\) and \(C_{i,j} = (c_{i,j})_{s,t}\) can be shown to have similar form to the matrix \(A_{j,k}\).

Similar to the alternating direction method for the classical integer-order PDE, in order to maintain the approximation order, it is necessary to provide the additional boundary values in the \(x\)-direction \(u_{0,j,k}^{n+1/3}, u_{N_1,j,k}^{n+1/3}\) and in the \(y\)-direction \(u_{i,0,k}^{n+2/3}, u_{i,N_2,k}^{n+2/3}\) when solving the system of equations with coefficient matrices \(A_{j,k}\) and \(B_{i,k}\). For example, we provide the additional boundary values \(u_{0,j,k}^{n+1/3}, u_{N_1,j,k}^{n+1/3}\) according to:

\[u_{i,j,k}^{n+1/3} = (1 + \mu_2 \delta_y^3)(1 + \mu_3 \delta_z^3)u_{i,j,k}^{n+1}, \quad i = 0, N_1, \tag{28}\]
where \( j = 1, \ldots, N_2 - 1 \), \( k = 1, \ldots, N_3 - 1 \), \( n = 0, 1, \ldots, N - 1 \), and 
\( u_{i,0,k}^{n+2/3}, u_{i,N_2,k}^{n+2/3} \) can be obtained from
\[
\begin{align*}
  u_{i,j,k}^{n+2/3} &= (1 + \mu_3 \delta_x^2) u_{i,j,k}^{n+1}, \quad j = 0, N_2, \quad (29)
\end{align*}
\]
where \( i = 1, \ldots, N_1 - 1 \), \( k = 1, \ldots, N_3 - 1 \), \( n = 0, 1, \ldots, N - 1 \).

From the three coefficient matrices, it can be seen that at each time step, we must solve, for each fixed \((j, k)\) (every layer in the \(x\)-direction) or each fixed \((i, k)\) (every layer in the \(y\)-direction) or each fixed \((i, j)\) (every layer in the \(z\)-direction) a linear system of equations with \(N_1 - 1\), or \(N_2 - 1\), or \(N_3 - 1\) unknowns.

4. Stability of FADM

In this section, we prove the stability of FADM for the ST-FBTE.

Let \( X = [x_1, x_2, \ldots, x_m]^T \in \mathbb{R}^m \), \( \|X\|_\infty = \max_{1 \leq i \leq m} |x_i| \).

**Lemma 5.** Let the matrix \( D = (d_{i,j})_{m \times m} \in \mathbb{R}^{m \times m} \) satisfy the conditions
\[
\sum_{l=1, l \neq i}^m |d_{i,l}| \leq |d_{i,i}| - 1, \quad (i = 1, 2, \ldots, m),
\]
then
\[
\|X\|_\infty \leq \|DX\|_\infty. \quad (30)
\]

**Proof.** See [21].

In order to prove the stability of FADM, we need to rewrite (23)-(26) in matrix form.

Utilizing (27), the linear system (24) may be written in matrix form as
\[
\begin{align*}
  A_{j,k} U_{j,k}^{n+1/3} &= \sum_{l=0}^{n-1} (b_l - b_{l+1}) U_{j,k}^{n-l} + b_n U_{j,k}^0 + \mu_0 F_{j,k}^{n+1} \\
  &\quad + (0, \cdots, 0, \mu_1 u_{N_1,j,k}^{n+1/3})^T, \quad (31)
\end{align*}
\]
where \( 1 \leq j \leq N_2 - 1 \), \( 1 \leq k \leq N_3 - 1 \), \( U_{j,k}^{n+1/3} = (u_{i,j,k}^{n+1/3}, u_{i+1,j,k}^{n+1/3}, \cdots, u_{i,N_1-1,j,k}^{n+1/3})^T \),
\( A_{j,k} = (a_{j,k})_{s,t} \), and \( F_{j,k}^{n+1} = (f_{j,k}^{n+1}, f_{j+1,k}^{n+1}, \cdots, f_{N_1-1,j,k}^{n+1})^T \).

Similarly, (25) may be written in matrix form as
\[
B_{i,k} U_{i,k}^{n+2/3} = U_{i,k}^{n+1/3} + (0, \cdots, 0, \mu_2 u_{i,N_2,k}^{n+2/3})^T, \quad (32)
\]
The FADM defined by (23) is unconditionally stable, and

From Lemma 4, it can be seen that

we have

Proof.

Thus, using mathematical induction, we have the following result:

**Theorem 1.** The FADM defined by (23) is unconditionally stable, and

\[ \| \varepsilon^{n+1} \|_\infty \leq \| \varepsilon^0 \|_\infty, \quad n = 0, 1, 2, \ldots. \]

**Proof.** From Lemma 4, it can be seen that \( A_{i,k}, B_{i,k}, \) and \( C_{i,j} \) satisfy the condition of Lemma 5. According to the relationship between the matrices \( S, T, \) and \( V \) and \( C_{i,j}, \) we see that \( S, T, \) and \( V \) also satisfy the condition of Lemma 5. Therefore, when \( n = 0, \) using Lemmas 3 and 5, we have

\[ \| \varepsilon^1 \|_\infty \leq \| V \varepsilon^1 \|_\infty \leq \| TV \varepsilon^1 \|_\infty \leq \| STV \varepsilon^1 \|_\infty = \| b_0 \varepsilon^0 \|_\infty = \| \varepsilon^0 \|_\infty. \]
Now, suppose that $\|\varepsilon^m\|_\infty \leq \|\varepsilon^0\|_\infty$, $m = 1, 2, \ldots, n$. Similarly, using Lemmas 3 and 5 again, we have

\[
\|V\varepsilon^{n+1}\|_\infty \leq \|TV\varepsilon^{n+1}\|_\infty \leq \|STV\varepsilon^{n+1}\|_\infty
= \left\| \sum_{l=0}^{n-1} (b_l - b_{l+1})\varepsilon^{n-l} + b_n\varepsilon^0 \right\|_\infty
\leq \sum_{l=0}^{n-1} (b_l - b_{l+1})\|\varepsilon^{n-l}\|_\infty + b_n\|\varepsilon^0\|_\infty
\leq \left( \sum_{l=0}^{n-1} (b_l - b_{l+1}) + b_n \right)\|\varepsilon^0\|_\infty
= \|\varepsilon^0\|_\infty.
\]

Hence the FADM defined by (23) is unconditionally stable.

5. Convergence of FADM

To prove the convergence of the FADM, we note that the time difference operator in (21) has a local truncation error of order $O(\tau^{2-\alpha})$, and the three space difference operators in (21) have local truncation errors of orders $O(h_x)$, $O(h_y)$ and $O(h_z)$, respectively, which was proved in [2]. The only remaining term in the local error of the FADM is the additional small term (22).

For any positive integer $l$, let $W_{l;1}(\mathbb{R}^3)$ denote the collection of all functions $f \in C^l(\mathbb{R}^3)$ whose partial derivatives up to order $l$ are in $L^1(\mathbb{R}^3)$ and whose partial derivatives up to order $l-1$ vanish at infinity [11].

From Definition 1, we have

\[
\frac{\partial^\beta}{\partial|x|^\alpha \partial|y|^\beta} u(x, y, z, t) = c_\beta^2 (0D_x^\beta + xD_{L_1}^\beta)(0D_y^\beta + yD_{L_2}^\beta)u(x, y, z, t)
= c_\beta^2 (0D_x^\beta 0D_y^\beta + 0D_x^\beta yD_{L_2}^\beta + xD_{L_1}^\beta 0D_y^\beta + xD_{L_1}^\beta yD_{L_2}^\beta)u(x, y, z, t),
\]

(36)

Let $r > 2\beta + 3$ be an integer, and integers $p, q \geq 0$, then for $f \in W^{l,1}(\mathbb{R}^3)$, we have (see Theorem 3.1 in [11])

\[
h_x^{-\beta}h_y^{-\beta}\sum_{n=0}^{\infty}\sum_{m=0}^{\infty} \omega_n \omega_m u(x-(n-p)h_x, y-(m-q)h_y, z, t)
= 0 D_x^\beta 0D_y^\beta u(x, y, z, t) + O(h_x + h_y)
\]

(37)
Similarly, we have
\[
\delta^3_y u^{n+1}_{i,j,k} = \left( \sum_{q=0}^{j+1} \omega_q u^{n+1}_{i,j-q+1,k} + \sum_{q=0}^{N_2-j+1} \omega_q u^{n+1}_{i,j+q+1,k} \right)
\]
\[
= \sum_{q=0}^{j+1} \omega_q \left( \sum_{p=0}^{i+1} \omega_p u^{n+1}_{i-p+1,j-q+1,k} + \sum_{p=0}^{N_1-i+1} \omega_p u^{n+1}_{i+p-1,j-q+1,k} \right)
+ \sum_{q=0}^{N_2-j+1} \omega_q \left( \sum_{p=0}^{i+1} \omega_p u^{n+1}_{i-p+1,j+q+1,k} + \sum_{p=0}^{N_1-i+1} \omega_p u^{n+1}_{i+p-1,j+q+1,k} \right)
\]
\[
= \sum_{p=0}^{i+1} \sum_{q=0}^{j+1} \omega_p \omega_q u^{n+1}_{i-p+1,j-q+1,k} + \sum_{p=0}^{N_1-i+1} \sum_{q=0}^{j+1} \omega_p \omega_q u^{n+1}_{i+p-1,j-q+1,k}
+ \sum_{p=0}^{i+1} \sum_{q=0}^{N_2-j+1} \omega_p \omega_q u^{n+1}_{i-p+1,j+q+1,k} + \sum_{p=0}^{N_1-i+1} \sum_{q=0}^{N_2-j+1} \omega_p \omega_q u^{n+1}_{i+p-1,j+q+1,k}.
\] (38)

With boundary condition (11), the solution function may be zero-extending for \( x < 0 \) or \( y < 0 \). According to (37), we have
\[
h_x^{-\beta} h_y^{-\beta} \sum_{p=0}^{i+1} \sum_{q=0}^{j+1} \omega_p \omega_q u^{n+1}_{i-p+1,j-q+1,k} = h_x^{-\beta} h_y^{-\beta} \sum_{p=0}^{\infty} \sum_{q=0}^{\infty} \omega_p \omega_q u^{n+1}_{i-p+1,j-q+1,k}
\]
\[
= 0 D_x^\beta \partial_y^\beta u(x_i, y_j, z_k, t_{n+1}) + O(h_x + h_y).
\] (39)

Similarly, we have
\[
h_x^{-\beta} h_y^{-\beta} \sum_{p=0}^{N_1-i+1} \sum_{q=0}^{j+1} \omega_p \omega_q u^{n+1}_{i+p-1,j-q+1,k} = x D_{L_1}^\beta \partial_y^\beta u(x_i, y_j, z_k, t_{n+1})
\]
\[
+ O(h_x + h_y),
\] (40)

\[
h_x^{-\beta} h_y^{-\beta} \sum_{p=0}^{i+1} \sum_{q=0}^{N_2-j+1} \omega_p \omega_q u^{n+1}_{i-p+1,j+q+1,k} = 0 D_x^\beta \partial_y^\beta u(x_i, y_j, z_k, t_{n+1})
\]
\[
+ O(h_x + h_y),
\] (41)

\[
h_x^{-\beta} h_y^{-\beta} \sum_{p=0}^{N_1-i+1} \sum_{q=0}^{N_2-j+1} \omega_p \omega_q u^{n+1}_{i+p-1,j+q+1,k} = x D_{L_1}^\beta \partial_y^\beta u(x_i, y_j, z_k, t_{n+1})
\]
\[
+ O(h_x + h_y).
\] (42)
Therefore, from (36), (39)-(42), we obtain
\[ \frac{\partial^\beta}{\partial |x|^\beta \partial |y|^\beta} u(x, y, z, t_{n+1}) = c_\beta^2 h_x^{-\beta} h_y^{-\beta} \delta_x^\beta \delta_y^\beta u_i,j,k^{n+1} + O(h_x + h_y). \] (43)

Thus, we have
\[ \mu_1 \mu_2 \delta_x^\beta \delta_y^\beta u_i,j,k^{n+1} = \frac{K_0^2 \tau^{2\alpha} \Gamma^2}{4 \alpha} \frac{\partial^\beta}{\partial |x|^\beta \partial |y|^\beta} u(x, y, z, t_{n+1}) + O(h_x + h_y) \]
\[ = \tau^\alpha O[\tau^\alpha (h_x + h_y)]. \] (44)

Similarly, we obtain
\[ \mu_1 \mu_3 \delta_x^\beta \delta_z^\beta u_i,j,k^{n+1} = \tau^\alpha O[\tau^\alpha (h_x + h_z)], \] (45)
\[ \mu_2 \mu_3 \delta_y^\beta \delta_z^\beta u_i,j,k^{n+1} = \tau^\alpha O[\tau^\alpha (h_y + h_z)], \] (46)
\[ \mu_1 \mu_2 \mu_3 \delta_x^\beta \delta_y^\beta \delta_z^\beta u_i,j,k^{n+1} = \tau^\alpha O[\tau^{2\alpha} (h_x + h_y + h_z)]. \] (47)

Together with (12)-(15) and (44)-(47), we have the following theorem.

**Theorem 2.** The FADM (23) is consistent to the ST-FBTE (9) with order \(O(\tau^{2-\alpha} + h_x + h_y + h_z)\).

Setting \( e_i,j,k^n = u(x, y, z, t_n) - u_i,j,k^n \), and let \( e^n = (e_{1,1,1}^n, e_{2,1,1}^n, \cdots, e_{N_1-1,N_2-1,N_3-1}^n)^T \),
then \( e^0 = 0 \).

From (12)-(15) and (44)-(47), the error \( e^n \) satisfies
\[ STV e^{n+1} = \sum_{l=0}^{n-1} (b_{l+1} - b_l) e^{n-l} + C_1 \tau^\alpha (\tau^{2-\alpha} + h_x + h_y + h_z). \] (48)

Thus, using mathematical induction, we have the following result:

**Theorem 3.** The FADM (23) is convergent, and there is a positive constant \( C^* \), such that
\[ \| e^{n+1} \|_\infty \leq C^* (\tau^{2-\alpha} + h_x + h_y + h_z). \] (49)
Proof. When \( n = 0 \), and using Lemmas 3, 4 and 5, we have

\[
\|e^1\|_\infty \leq \|Ve^1\|_\infty \leq \|TVe^1\|_\infty \leq \|STVe^1\|_\infty = C_1\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z).
\]

Now, suppose that

\[
\|e^m\|_\infty \leq C_1b_{m-1}^{-1}\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z),
\]

where \( m = 1, 2, \ldots, n \). Using Lemmas 3, 4 and 5 again, we have

\[
\|e^{n+1}\|_\infty \leq \|Ve^{n+1}\|_\infty \leq \|TVe^{n+1}\|_\infty \leq \|STVe^{n+1}\|_\infty
\]

\[
= \sum_{l=0}^{n-1} (b_l - b_{l+1})e^{n-l} + C_1\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z) + C_1\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z)
\]

\[
\leq \sum_{l=0}^{n-1} (b_l - b_{l+1})C_1b_{n-l-1}^{-1}\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z)
\]

\[
+ C_1\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z)
\]

\[
\leq \sum_{l=0}^{n-1} (b_l - b_{l+1})C_1b_n^{-1}\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z)
\]

\[
+ C_1\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z)
\]

\[
= C_1b_n^{-1}\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z).
\]

We note that

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

and there exists a positive constant \( C_2 \), such that

\[
\|e^{n+1}\|_\infty \leq C_1C_2n^\alpha\tau^\alpha(\tau^{2-\alpha} + h_x + h_y + h_z).
\]

Finally, note that \( n\tau \leq T \) is finite, so there exists a positive constant \( C^* \), such that

\[
\|e^{n+1}\|_\infty \leq C^*(\tau^{2-\alpha} + h_x + h_y + h_z) \text{ for } n = 0, 1, 2, \ldots.
\]

Hence the FADM (23) is convergent.

6. Numerical results

In order to better present the efficiency of the fractional alternating direction method, we first show a two-dimensional example to confirm our
theoretical analysis. The machine we used to perform the numerical tests in
this section is a laptop Lenovo Y430.

In Example 1, we use the same example in [2] for comparison.

Example 1. The following space and time fractional Bloch-Torrey equa-
tion with initial and boundary conditions on a finite domain is considered
(See [2]):

\[ K_\alpha C D_t^\alpha M(r, t) = K_\beta \left( \frac{\partial^\beta}{\partial |r|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} \right) M(r, t) + f(r, t), \quad (50) \]

\[ M(r, 0) = 0, \quad (51) \]

\[ M(r, t)|_\Gamma = 0, \quad (52) \]

where

\[ f(r, t) = \frac{K_\beta t^{\alpha+\beta}}{2 \cos(\beta \pi/2)} \left\{ \frac{2}{\Gamma(3-\beta)} [x^{2-\beta} + (1-x)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)} [x^{3-\beta} + (1-x)^{3-\beta}] \right. \]

\[ + (1-x)^{3-\beta} + \frac{24}{\Gamma(5-\beta)} [x^{4-\beta} + (1-x)^{4-\beta}] y^2 (1-y)^2 \]

\[ + \frac{2}{\Gamma(3-\beta)} [y^{2-\beta} + (1-y)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)} [y^{3-\beta} + (1-y)^{3-\beta}] \]

\[ + \frac{24}{\Gamma(5-\beta)} [y^{4-\beta} + (1-y)^{4-\beta}] x^2 (1-x)^2 \left\} \right. \]

\[ + \frac{K_\alpha \Gamma(\alpha+\beta+1)}{\Gamma(\beta+1)} t^\beta x^2 (1-x)^2 y^2 (1-y)^2, \quad (53) \]

and \( 0 < \alpha \leq 1, 1 < \beta \leq 2, t > 0, \ r = (x, y) \in \Omega, \ \Omega \) is the finite rectangular
region \([0,1] \times [0,1]\) and \( \Gamma \) is the boundary of \( \Omega \).

The exact solution of this problem is \( M(r, t) = t^{\alpha+\beta} x^2 (1-x)^2 y^2 (1-y)^2 \),
which can be verified by substituting directly into (50).

We take \( K_\alpha = 1.0, K_\beta = 0.5, \alpha = 0.8, \) and \( \beta = 1.8 \). Table 1 list-
s the CPU time calculated by a two-dimensional fractional alternating di-
rection method (2D-FADM), a two-dimensional implicit numerical scheme
(M1) [2] that is first order accuracy in space, and a two-dimensional im-
licit numerical method (M2) [22] that is second order accuracy in space
at time \( t = 1.0 \), where the temporal step \( \tau = 1/100 \) and spatial steps
\( h_x = h_y = 1/8, 1/16, 1/32 \). In Table 1, G-E, J and G-S signify the use
of Gauss elimination, Jacobi iteration and Gauss-Seidel iteration for M1 or
M2, respectively. A brief description of 2D-FADM, M1 and M2 is presented
in the Appendix.
Table 1: Comparison of CPU time (seconds) between 2D-FADM, M1 and M2 with temporal step $\tau = 1/100$ at time $t = 1.0$

<table>
<thead>
<tr>
<th>$h_x = h_y$</th>
<th>2D-FADM</th>
<th>M1</th>
<th>M2</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\frac{1}{8}$</td>
<td>0.15</td>
<td>5.52</td>
<td>3.86</td>
</tr>
<tr>
<td>$\frac{1}{16}$</td>
<td>0.32</td>
<td>28.06</td>
<td>12.77</td>
</tr>
<tr>
<td>$\frac{1}{32}$</td>
<td>2.58</td>
<td>1356.33</td>
<td>63.05</td>
</tr>
</tbody>
</table>

From Table 1 it can be seen that the use of direct methods to solve the traditional implicit numerical schemes for these fractional-in-space models are extremely time-consuming compared with using indirect methods. In fact there is a more than 20 fold reduction in computing time when the Gauss-Seidel method is employed for the smaller mesh size of $h_x = h_y = 1/32$. One notes that even though the fractional alternating direction method requires the solution of smaller dense matrices of much reduced dimension using direct methods at each cycle, it is still more computationally efficient than these classical iterative strategies, with greatly reduced CPU time for all mesh sizes. In particular, the reduction in CPU time for the FADM is even more significant for smaller mesh sizes. One observes for the smaller mesh $h_x = h_y = 1/32$ a 20 fold reduction in CPU time over the Gauss-Seidel method. The fractional alternating direction method is clearly the most efficient of the methods investigated here for solving the large fractional-in-space linear systems.

We now exhibit in Example 2 the application of FADM on the space and time fractional Bloch-Torrey equation in 3-D with initial and boundary conditions on a finite domain.

**Example 2.** The following space and time fractional Bloch-Torrey equation in 3-D with initial and boundary conditions on a finite domain is considered:

$$K_\alpha \mathcal{C} D_t^\alpha M(\mathbf{r}, t) = K_\beta \left( \frac{\partial^\beta}{\partial |x|^\beta} + \frac{\partial^\beta}{\partial |y|^\beta} + \frac{\partial^\beta}{\partial |z|^\beta} \right) M(\mathbf{r}, t) + f(\mathbf{r}, t), \quad (54)$$

$$M(\mathbf{r}, 0) = 0, \quad (55)$$

$$M(\mathbf{r}, t)|_{\Gamma} = 0, \quad (56)$$
Table 2: Comparison of CPU time and maximum error for FADM with temporal step \( \tau = 1/100 \) at time \( t = 1.0 \)

<table>
<thead>
<tr>
<th>( h_x = h_y = h_z )</th>
<th>Maximum error</th>
<th>CPU time(seconds)</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \frac{1}{4} )</td>
<td>0.003750</td>
<td>0.12</td>
</tr>
<tr>
<td>( \frac{1}{8} )</td>
<td>0.001267</td>
<td>0.55</td>
</tr>
<tr>
<td>( \frac{1}{16} )</td>
<td>0.0003537</td>
<td>6.63</td>
</tr>
<tr>
<td>( \frac{1}{32} )</td>
<td>0.0001675</td>
<td>121.29</td>
</tr>
</tbody>
</table>

where

\[
f(r, t) = \frac{K_\beta t^{\alpha+\beta}}{2\cos(\beta\pi/2)} \left\{ \left( \frac{2}{\Gamma(3-\beta)}[x^{2-\beta} + (1-x)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)}[x^{3-\beta}] \right) + (1-x)^{3-\beta} + \frac{24}{\Gamma(5-\beta)}[x^{4-\beta} + (1-x)^{4-\beta}]y^2(1-y)^2z^2(1-z)^2 \right. \\
\left. \left[ \frac{2}{\Gamma(3-\beta)}[y^{2-\beta} + (1-y)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)}[y^{3-\beta} + (1-y)^{3-\beta}] \right] + \frac{24}{\Gamma(5-\beta)}[y^{4-\beta} + (1-y)^{4-\beta}]x^2(1-x)^2z^2(1-z)^2 \right. \\
\left. + \left( \frac{2}{\Gamma(3-\beta)}[z^{2-\beta} + (1-z)^{2-\beta}] - \frac{12}{\Gamma(4-\beta)}[z^{3-\beta} + (1-z)^{3-\beta}] \right) + \frac{24}{\Gamma(5-\beta)}[z^{4-\beta} + (1-z)^{4-\beta}]x^2(1-x)^2y^2(1-y)^2 \right\} \\
+ \frac{K_\alpha \Gamma(\alpha + \beta + 1)}{\Gamma(\beta + 1)} t^\beta x^2(1-x)^2y^2(1-y)^2z^2(1-z)^2,
\]

and \( 0 < \alpha \leq 1, \ 1 < \beta \leq 2, \ t > 0, \ r = (x, y, z) \in \Omega, \ \Omega \) is the finite region \([0, 1] \times [0, 1] \times [0, 1]\) and \( \Gamma \) is the boundary of \( \Omega \).

The exact solution of this problem is \( M(r, t) = t^{\alpha+\beta}x^2(1-x)^2y^2(1-y)^2z^2(1-z)^2 \), which can be verified by substituting directly into (54).

In this example, we take \( K_\alpha = 1.0, K_\beta = 0.5, \alpha = 0.8, \) and \( \beta = 1.8 \). The fractional alternating direction implicit scheme, which is presented in Section 3, is used to solve this problem. Table 2 lists the CPU time and the maximum absolute error between the exact solution and the numerical solutions obtained by FADM at time \( t = 1.0 \), where the temporal step \( \tau = 1/100 \) and spatial steps \( h_x = h_y = h_z = 1/4, 1/8, 1/16, 1/32 \).
From Table 2, it can be seen that for the same spatial step, the FADM is convergent, which is consistent with our theoretical findings. We also note that although the 3D-INS implicit scheme could not be run on the laptop Lenovo Y430 due to its memory requirements, FADM was successful. However, this method still required considerable CPU time to obtain the 3-D solution.

We now exhibit in Example 3 the result of FADM for the space and time fractional Bloch-Torrey equation with a cubic nonlinear source term.

**Example 3.** The following space and time fractional Bloch-Torrey equation in 3-D with initial and boundary conditions on a finite domain is considered:

\[
K_\alpha C_0^t D_t^\beta M(r, t) = K_\beta \left( \frac{\partial^\beta}{\partial |x|^{\beta}} + \frac{\partial^\beta}{\partial |y|^{\beta}} + \frac{\partial^\beta}{\partial |z|^{\beta}} \right) M(r, t) + f(M, r, t), \tag{57}
\]

where the nonlinear source term is \( f(M, r, t) = M(M, r, t) - M^3(M, r, t) \), and \( 0 < \alpha \leq 1, 1 < \beta \leq 2, t > 0, r = (x, y, z) \in \Omega, \Omega \) is the finite cubic region \([0, 1] \times [0, 1] \times [0, 1]\) and \( \Gamma \) is the boundary of \( \Omega \).

The solution profiles of (57) by FADM, with spatial and temporal steps \( h_x = h_y = h_z = 1/50, \tau = 1/80 \) at \( z = 0.5 \) with \( \alpha = 0.8, \beta = 1.8, K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 0.2 \) for different \( t \) are exhibited in Figure 1. One can observe that the solution profile flattens as time increases.

Figure 2 shows the numerical solutions of ST-FBTE using FADM with spatial and temporal steps \( h_x = h_y = h_z = 1/50, \tau = 1/80 \) at time \( t = 0.1 \) and \( z = 0.5 \) with \( \alpha = 0.8, \beta = 1.8, K_\alpha = 1.0, t_{final} = 0.2 \) for different \( K_\beta \). From Figure 2, it can be seen that the coefficient \( K_\beta \) impacts on the solution profiles of (57), whereby a larger value of \( K_\beta \) produces more diffuse profiles.

In Figure 3, we illustrate the effect of the fractional order in space for this problem, with spatial and temporal steps \( h_x = h_y = h_z = 1/50, \tau = 1/80 \) at time \( t = 0.1 \) and \( z = 0.5 \) with \( K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 0.2 \) for \( \beta \) fixed at 1.8 and \( \alpha \) varying. One observes that as the fractional-in-time index is reduced the diffusion becomes more pronounced.

In Figure 4, we illustrate the effect of the fractional order in time for this problem, with spatial and temporal steps \( h_x = h_y = h_z = 1/50, \tau = 1/80 \) at time \( t = 0.1 \) and \( z = 0.5 \) with \( K_\alpha = 1.0, K_\beta = 1.0, t_{final} = 0.2 \) for \( \alpha \) fixed at 0.8 and \( \beta \) varying. Again we see the pronounced diffusion as \( \beta \) is decreased.
7. Conclusions

In this paper, a fractional alternating direction method (FADM) for solving the space and time fractional Bloch-Torrey equation (ST-FBTE) in 3-D has been derived. We prove that the FADM is unconditionally stable and convergent. We have used our numerical method to simulate a problem of practical importance involving a nonlinear source term. In all cases we conclude that the FADM is more computationally efficient than the standard implicit techniques solved using either direct or indirect methods, because
Figure 3: A plot of numerical solutions of ST-FBTE using FADM with spatial and temporal steps $h_x = h_y = h_z = 1/50$, $\tau = 1/80$ at time $t = 0.1$ and $z = 0.5$ with $K_\alpha = 1.0$, $K_\beta = 1.0$, $t_{final} = 0.2$ for $\beta$ fixed at 1.8. (a) $\alpha = 1.0$. (b) $\alpha = 0.95$. (c) $\alpha = 0.9$. (d) $\alpha = 0.8$.

the computational expense associated with the solution of the large dense matrix that is generated as a result of the three-dimensional discretisation is avoided.

Acknowledgments

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Figure 4: A plot of numerical solutions of ST-FBTE using FADM with spatial and temporal steps $h_x = h_y = h_z = 1/50$, $\tau = 1/80$ at time $t = 0.1$ and $z = 0.5$ with $K_\alpha = 1.0$, $K_\beta = 1.0$, $t_{final} = 0.2$ for $\alpha$ fixed at 0.8. (a) $\beta = 2.0$. (b) $\beta = 1.95$. (c) $\beta = 1.9$. (d) $\beta = 1.8$.

8. Appendix

(i) Two-dimensional implicit numerical scheme (M1) [2]:

$$u_{i,j}^{n+1} + \mu_1 \left( \sum_{p=0}^{i+1} \omega_p u_{i-p+1,j}^{n+1} + \sum_{p=0}^{N_1-i+1} \omega_p u_{i+p-1,j}^{n+1} \right) + \mu_2 \left( \sum_{q=0}^{j+1} \omega_q u_{i,j-q+1}^{n+1} \right) + \sum_{q=0}^{N_2-j+1} \omega_q u_{i,j+q-1}^{n+1} = \sum_{l=0}^{n-1} (b_l - b_{l+1}) u_{i,j}^{n-l} + b_n u_{i,j}^0 + \mu_0 f_{i,j}^{n+1},$$

$$i = 1, 2, \cdots, N_1 - 1, j = 1, 2, \cdots, N_2 - 1,$$
with
\begin{align*}
  u_{i,j}^0 &= g_{i,j} = g(x_i, y_j), \\
  u_{0,j}^{n+1} &= u_{N_1,j}^{n+1} = u_{i,0}^{n+1} = u_{i,N_2}^{n+1} = 0, \\
  (i = 0, 1, \cdots, N_1, j = 0, 1, \cdots, N_2)
\end{align*}

where \( \mu_0 = \frac{\tau^n (2-\alpha)}{K_\alpha}, \mu_1 = \frac{c_3 K_\alpha \tau^n (2-\alpha)}{K_\alpha h_x^2}, \mu_2 = \frac{c_3 K_\alpha \tau^n (2-\alpha)}{K_\alpha h_y^2}, \)
and noting that coefficients \( \mu_0 > 0, \mu_1, \mu_2 < 0 \) for \( 0 < \alpha \leq 1 \) and \( 1 < \beta \leq 2. \)

(ii) Two-dimensional fractional alternating direction method (2D-FADM):
\begin{align*}
(1 + \mu_1 \delta_x)u_{i,j}^{n+1/2} &= \sum_{l=0}^{n-1} (b_l - b_{l+1})u_{i,j}^{n-l} + b_n u_{i,j}^0 + \mu_0 f_{i,j}^{n+1}, \\
(1 + \mu_2 \delta_y)u_{i,j}^{n+1} &= u_{i,j,k}^{n+1/2},
\end{align*}

where
\begin{align*}
  \delta_x u_{i,j}^{n+1} &= \sum_{p=0}^{i+1} \omega_p u_{i-p+1,j}^{n+1} + \sum_{p=0}^{N_1-i+1} \omega_p u_{i+p-1,j}^{n+1}, \\
  \delta_y u_{i,j}^{n+1} &= \sum_{q=0}^{j+1} \omega_q u_{i,j-q+1}^{n+1} + \sum_{q=0}^{N_2-j+1} \omega_q u_{i,j+q-1}^{n+1}.
\end{align*}

The additional boundary values \( u_{0,j}^{n+1/2}, u_{N_1,j}^{n+1/2}, \) which can be obtained as
\[ u_{i,j}^{n+1/2} = (1 + \mu_2 \delta_y)u_{i,j}^{n+1}, \quad i = 0, N_1, \]
where \( j = 1, \cdots, N_2 - 1, n = 0, 1, \cdots, N - 1. \)

(iii) Two-dimensional implicit numerical method (M2) [22]:
\begin{align*}
  u_{i,j}^{n+1} &= \mu_1 \sum_{p=-N_1+i}^{i} \omega_p u_{i-p,j}^{n+1} + \mu_2 \sum_{q=-N_2+j}^{j} \omega_q u_{i,j-q}^{n+1} \\
  &= \sum_{l=0}^{n-1} (b_l - b_{l+1})u_{i,j}^{n-l} + b_n u_{i,j}^0 + \mu_0 f_{i,j}^{n+1}, \\
  i = 1, \cdots, N_1 - 1, j = 1, 2, \cdots, N_2 - 1,
\end{align*}
with

\[
\begin{align*}
    u^0_{i,j} &= g_{i,j} = g(x_i, y_j), \\
    u^{n+1}_{0,j} &= u^{n+1}_{N_1,j} = u^{n+1}_{i,0} = u^{n+1}_{i,N_2}, \\
    (i &= 0, 1, \ldots, N_1, j = 0, 1, \ldots, N_2)
\end{align*}
\]

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

References


