An implicit numerical method for the space-time variable-order fractional Bloch-Torrey equation

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Abstract. Recently, a new space-time fractional Bloch-Torrey equation (ST-FBTE) has been proposed to study anomalous diffusion in the human brain. In a paper, we consider the ST-FBTE with variable fractional order derivatives. The time and space derivatives are replaced by the variable-order Caputo and variable-order Riesz fractional derivatives, respectively. An implicit numerical method for the equation are proposed. Unconditional stability and a special case convergence of the proposed method are proved by the mathematical induction. Some numerical examples are given to support our theoretical analysis.

1. Introduction
In a paper, we study the space-time variable-order fractional Bloch-Torrey equation (ST-VO-FBTE) which is stated as follows

\[
\begin{cases}
\partial_t^\alpha u(x,t) = \kappa(x,t) \partial_\|x\|^\beta u(x,t) + f(x,t), \quad (x,t) \in \Omega = (a,b) \times (0,T], \\
u(x,0) = \phi(x), \quad a \leq x \leq b, \\
u(a,t) = 0, \nu(b,t) = 0, \quad 0 \leq t \leq T,
\end{cases}
\]

where \(0 < \alpha \leq \alpha(x,t) \leq \bar{\alpha} \leq 1\) and \(1 < \beta \leq \beta(x,t) \leq \bar{\beta} \leq 2\), \(\kappa(x,t)\) stands for the generalized diffusion coefficient, \(\partial_t^\alpha u(x,t)\) denotes Caputo fractional derivative of variable-order \(\alpha(x,t)\) to the function \(u(x,t)\), the notation \(\partial_\|x\|^\beta u(x,t)/\partial_\|x\|^\beta\) presents the generalized Riesz fractional derivative of variable-order \(\beta(x,t)\) to function \(u(x,t)\), which has introduced in the literature of [1] and [2], but for readability, we restate it in the following

\[
\frac{\partial^\beta(x,t) u(x,t)}{\partial \|x\|^\beta} = -\frac{1}{\cos(\beta(x,t)\pi/2)}(\rho_a D^\beta(x,t) + \sigma_b D^\beta(x,t))u(x,t),
\]

in which \(a D^\beta(x,t) u(x,t)\) and \(b D^\beta(x,t) u(x,t)\) represent the left-side and right-side variable-order Riemann-Liouville fractional derivative to the function, respectively, defined by

\[
a D^\beta(x,t) u(x,t) = \frac{1}{\Gamma(2-\beta(x,t))} \int_a^x (\theta - \xi)^{1-\beta(x,t)} u(\xi,t) d\xi |_{\theta=x},
\]

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Hence, the previous equation can be expressed by the next matrix form

\[ xD_x^\beta(x,t)u(x,t) = \frac{1}{\Gamma(2 - \beta(x,t))} \frac{d^2}{d\theta^2} \int_{\theta}^{b} (\xi - \theta)^{1-\beta(x,t)}u(\xi, t)d\xi |_{\theta=x}. \]

Finally, in order to simplify the process in the sequel, we set \( A(x, t) = \kappa(x, t) \times \left( -\cos \beta(x,t) \pi / 2 \right) \) \((A(x, t) > 0)\) to conclude the section.

2. Implicit numerical method for the ST-VO-FBTE

In this section, we shall derive a numerical approximation of Eq.(1). To this end, we let \( h = (b - a)/m \) and \( \tau = T/n \) as the spatial step and temporal step, respectively, moreover, using \( u_i^k \) as the numerical approximation to \( u(x_i, t_k) \), and similar for \( \alpha_i^k = \alpha(x_i, t_k), \beta_i^k = \beta(x_i, t_k) \) and \( f_i^k = f(x_i, t_k) \).

Thus, suppose \( u \in C^{(2)}(\Omega) \), adopting the discrete scheme given in [4], we may discretize the variable order time fractional derivative by

\[
e_0 D_t^{\alpha_i^{k+1}} u(x_i, t_{k+1}) = \frac{\tau^{-\alpha_i^{k+1}}}{\Gamma(2 - \alpha_i^{k+1})} \sum_{j=0}^{k} ((u(x_i, t_{k+1-j}) - u(x_i, t_k - j))) b_i^{k+1,j} + O(\tau). \tag{2}
\]

In what follow, by letting \( r_i^{k+1} = \tau^{\alpha_i^{k+1}} \Gamma(2 - \alpha_i^{k+1}), A_i^k = A(x_i, t_k) \) and \( b_i^{k,j} = (j+1)^{-1}\alpha_i^k - j^{1-\alpha_i^k} \). Combining (2) and Lemma 3.1 of [2], we can discrete (1) by the following implicit difference scheme:

\[
[1 - r_i^1 A_i^1(\rho h^{-\beta_i^{k+1}} g_i^{1}_{\beta_i^{k+1}} + \sigma h^{-\beta_i^{k+1}} g_i^{1}_{\beta_i^{k+1}})]u_i^1 - r_i^1 A_i^1(\rho h^{-\beta_i^{k+1}} \sum_{j=0,j\neq 1}^{i+1} g_j^{1}_{\beta_i^{k+1}} u_j^{1,i+1-j}) + \sigma h^{-\beta_i^{k+1}} \sum_{j=0,j\neq 1}^{m-i+1} g_j^{1}_{\beta_i^{k+1}} u_j^{1,i+1-j}) = u_i^0 + r_i^1 f_i^1, \tag{3}
\]

\[
[1 - r_i^{k+1} A_i^{k+1}(\rho h^{-\beta_i^{k+1}} g_i^{1}_{\beta_i^{k+1}} + \sigma h^{-\beta_i^{k+1}} g_i^{1}_{\beta_i^{k+1}})]u_i^{k+1} - r_i^{k+1} A_i^{k+1}(\rho h^{-\beta_i^{k+1}} \sum_{j=0,j\neq 1}^{k+1} g_j^{1}_{\beta_i^{k+1}} u_j^{1,i+1-j}) + \sigma h^{-\beta_i^{k+1}} \sum_{j=0,j\neq 1}^{m-i+1} g_j^{1}_{\beta_i^{k+1}} u_j^{1,i+1-j}) = \sum_{j=0}^{k-1} (b_j^{k+1,i} - b_j^{k+1,i+1}) u_j^{k+1,i} + b_j^{k+1,i} u_j^{0,i} + r_i^{k+1} f_i^{k+1}, \tag{4}
\]

in which \( i = 1, 2, \ldots, m - 1; k = 1, 2, \ldots, n - 1 \).

The initial and boundary conditions are discretized as

\[
u_i^0 = \phi(ih), \ i = 0, 1, 2, \ldots, m, \quad u_m^k = 0, \quad \text{and} \quad u_m^k = 0, \quad k = 0, 1, 2, \ldots, n. \tag{5}\]

Hence, the previous equation can be expressed by the next matrix form

\[
\begin{cases}
W^{1}U^1 = U^0 + r^1 f^1, \\
W^{K+1}U^{K+1} = \sum_{j=0}^{k-1} (b_j^{k+1,i} - b_j^{k+1,i+1}) U^{k-j} + b_j^{k+1,i} U^0 + r^{k+1} f^{k+1}, \\
U^0 = \phi.
\end{cases}
\]

in which \( U^k = (u_1^k, u_2^k, \ldots, u_m^k)^T, b_j^k = (b_1^{k,j}, b_2^{k,j}, \ldots, b_{m-1,j})^T, r^k = (r_1^k, r_2^k, \ldots, r_{m-1}^k)^T, f^k = \ldots \)
\( (f^k_1, f^k_2, \ldots, f^k_{m-1})^T, \phi = (\phi_1, \phi_2, \ldots, \phi_{m-1})^T, \) and \( W^k = (w^k_{ij}) : \)

\[
\begin{align*}
  w^k_{ij} &= \begin{cases}
    -r^k_i A^k_i \sigma h^{-\beta^k_{i-1}} g^0_{\beta^k_{i-1}} + \sigma h^{-\beta^k_{i-1}} g^2_{\beta^k_{i-1}}, & j \geq i + 2 \\
    -r^k_i A^k_i (\rho h^{-\beta^k_{i+1}} g^0_{\beta^k_{i+1}} + \sigma h^{-\beta^k_{i-1}} g^2_{\beta^k_{i-1}}), & j = i + 1 \\
    1 - r^k_i A^k_i (\rho h^{-\beta^k_{i+1}} g^0_{\beta^k_{i+1}} + \sigma h^{-\beta^k_{i-1}} g^1_{\beta^k_{i-1}}), & j = i \\
    -r^k_i A^k_i (\rho h^{-\beta^k_{i+1}} g^2_{\beta^k_{i+1}} + \sigma h^{-\beta^k_{i-1}} g^0_{\beta^k_{i-1}}), & j = i - 1 \\
    -r^k_i A^k_i \rho h^{-\beta^k_{i+1}} g^{i-j+1}_{\beta^k_{i+1}}, & j \leq i - 2,
  \end{cases}
\end{align*}
\]

for \( i = 1, 2, \ldots, m - 1, j = 1, 2, \ldots, m - 1, k = 1, 2, \ldots, n. \)

In accordance with Lemma 3 of [3], which associated with (6) to see that the matrix \( W \) is strictly diagonally dominant with positive diagonal terms and nonpositive off-diagonal terms. Hence, finally, the following theorem is established.

**Theorem 2.1.** The discretization matrix \( W \) is invertible. Furthermore, the system (3)-(5) has a unique solution.

### 3. Stability and Convergence of the Implicit numerical method

**Theorem 3.1.** The implicit difference scheme (3)-(5) is unconditionally stable.

**Proof.** Suppose that \( \tilde{u}^k_i \) is the approximate solution of \( u^k_i \), which is the exact solution of the implicit scheme (3) and (4). The error \( e^k_i = \tilde{u}^k_i - u^k_i \), satisfies

\[
[1 - r^1_i A^1_i (\rho h^{-\beta^1_{i+1}} g^0_{\beta^1_{i+1}} + \sigma h^{-\beta^1_{i-1}} g^1_{\beta^1_{i-1}})] e^1_i - r^1_i A^1_i (\rho h^{-\beta^1_{i+1}} g^0_{\beta^1_{i+1}}) \sum_{j=0,j \neq 1}^{i+1} g^j_{\beta^1_{i+1}} e^1_{i+j} = \varepsilon^0_1,
\]

\[
[1 - r^{k+1}_i A^{k+1}_i (\rho h^{-\beta^{k+1}_{i+1}} g^0_{\beta^{k+1}_{i+1}} + \sigma h^{-\beta^{k+1}_{i-1}} g^1_{\beta^{k+1}_{i-1}})] e^{k+1}_i - r^{k+1}_i A^{k+1}_i (\rho h^{-\beta^{k+1}_{i+1}} g^0_{\beta^{k+1}_{i+1}}) \sum_{j=0,j \neq 1}^{i+1} g^j_{\beta^{k+1}_{i+1}} e^{k+1}_{i+j} = \varepsilon^{k+1}_i,
\]

Next, we let \( \| X^1 \|_\infty = |e^1_i| = \max_{1 \leq i \leq m-1} |e^1_i| \) and notice that \( \sum_{j=0}^{l} g^j_{\beta^1_{i+1}} < 0 \), thus

\[
\| X^1 \|_\infty = |e^1_i| \leq |e^1_i| - r^1_i A^1_i (\rho h^{-\beta^1_{i+1}} \sum_{j=0}^{l} g^j_{\beta^1_{i+1}} |e^1_i| + \sigma h^{-\beta^1_{i-1}} \sum_{j=0}^{m-l-1} g^j_{\beta^1_{i-1}} |e^1_i|)
\]

\[
\leq |1 - r^1_i A^1_i (\rho h^{-\beta^1_{i+1}} g^0_{\beta^1_{i+1}} + \sigma h^{-\beta^1_{i-1}} g^1_{\beta^1_{i-1}})] e^1_i - r^1_i A^1_i (\rho h^{-\beta^1_{i+1}} g^0_{\beta^1_{i+1}}) \sum_{j=0,j \neq 1}^{i+1} g^j_{\beta^1_{i+1}} e^{1}_{i+j} + |\| e^0_1 | \leq \| X^0 \|_\infty .
\]
In what follow, in view of \( \|X^{k+1}\|_\infty = |\varepsilon_i^{k+1}| = \max_{1 \leq i \leq m-1} |\varepsilon_i^{k+1}| \) and assume that 
\( \|X^j\|_\infty \leq \|X^0\|_\infty (j \leq k) \), together with Lemma 3 of [3] and Lemma 1 of [4] to see that 
\[
\|X^{k+1}\|_\infty = |\varepsilon_i^{k+1}| \leq |\varepsilon_i^{k+1}| - r_l^{k+1} A_{l+1}^{k+1}(\rho h^{\beta_{l+1}} | g_{l+1}^{j+1} | \varepsilon_{i+1}^{k+1} | + \sigma h^{-\beta_{l+1}} \sum_{j=0}^{m-l+1} g_{l+1}^{j+i} | \varepsilon_i^{k+1} |)
\]
\[
\leq \sum_{j=0}^{k-1} \left( k_{i,j}^{k+1} - b_{i,j}^{k+1} \right) |\varepsilon_i^{k-j}| + b_{i,k}^{k+1} | \varepsilon_i^{0}| \leq \sum_{j=0}^{k-1} \left( b_{i,j}^{k+1} - b_{l,j}^{k+1} \right) \|X^{k-j}\|_\infty + b_{l,k}^{k+1} \|X^0\|_\infty
\]
\[
\leq \sum_{j=0}^{k-1} \left( b_{i,j}^{k+1} - b_{l,j}^{k+1} \right) \|X^0\|_\infty + b_{l,k}^{k+1} \|X^0\|_\infty = \|X^0\|_\infty.
\]
Therefore, the implicit difference scheme defined by (3)-(5) is unconditionally stable.

In what follows, we study a special case of discrete scheme (3)-(5) for the time fractional derivatives is independent of time variable \( t \).

**Theorem 3.2.** Suppose that \( u^k_i \ (i = 1, 2, \ldots, m-1, k = 1, 2, \ldots, n) \) is the approximation solution of \( u(x,t_k) \) computed by scheme (3)-(5), then there exist a positive constant \( C \) independent of \( \tau \) and \( h \), such that 
\[
\|u(\cdot, t_k) - u^k\|_\infty \leq C(\tau + h),
\]

**Proof.** Firstly, denote \( u(x,t_k)(i = 1, 2, \ldots, m-1; k = 1, 2, \ldots, n) \) by the exact solution of \( \text{Eq.}(1) \) at mesh point \( (x_i, t_k) \) and define that \( u_i^k = u(x_i, t_k) - u_i^k, \ Y^k = (\eta_1^k, \eta_2^k, \ldots, \eta_{m-1}^k)^T. \)

Using \( Y^0 = 0 \), and \( u_i^k = u(x_i, t_k) - \eta_i^k \), it follows from (3) and (4) to get that 
\[
[1 - r_i A_i^1(\rho h^{-\beta_{i+1}} g_{i+1}^{1} + \sigma h^{-\beta_{i+1}} g_{i+1}^{1})] \eta_i^1 - r_i A_i^1(\rho h^{-\beta_{i+1}} \sum_{j=0}^{i+1} g_{i+1}^j \eta_i^{1+j}) + \sigma h^{-\beta_{i+1}} \sum_{j=0}^{i+1} g_{i+1}^j \eta_i^{1+j} = R_i^1,
\]
\[
[1 - r_i A_i^1(\rho h^{-\beta_{i+1}} g_{i+1}^{1} + \sigma h^{-\beta_{i+1}} g_{i+1}^{1})] \eta_i^k - r_i A_i^1(\rho h^{-\beta_{i+1}} \sum_{j=0}^{k-1} g_{i+1}^j \eta_i^{k+j}) + \sigma h^{-\beta_{i+1}} \sum_{j=0}^{k-1} g_{i+1}^j \eta_i^{k+j} = R_i^k,
\]
in which \( \alpha_i = \alpha(x_i), b_{i,j} = (j + 1)^{1-\alpha_i} - j^{1-\alpha_i} \), and \( r_i = \tau_{\alpha_i} \Gamma(2-\alpha_i). \)

According to the formula (2) and Lemma 3.1 of [2], it is easy to obtain that the truncation error \( R_i^k \) satisfies 
\( \|R_i^k\| \leq C \tau^{\alpha_i}(\tau + h), \ i = 1, 2, \ldots, m-1, k = 1, 2, \ldots, n. \)

Next, letting \( \|Y^1\|_\infty = |\eta_i^1| = \max_{1 \leq i \leq m-1} |\eta_i^1| \) and by calculating, we have 
\[
\|Y^1\|_\infty = |\eta_i^1| \leq |\eta_i^k| - r_i A_i^1(\rho h^{-\beta_{i+1}} \sum_{j=0}^{i+1} g_{i+1}^j | \eta_i^{1+j} | + \sigma h^{-\beta_{i+1}} \sum_{j=0}^{m-i} g_{i+1}^j | \eta_i^0 |)
\]
\[
\leq |1 - r_i A_i^1(\rho h^{-\beta_{i+1}} g_{i+1}^{1} + \sigma h^{-\beta_{i+1}} g_{i+1}^{1})| - r_i A_i^1(\rho h^{-\beta_{i+1}} \sum_{j=0}^{i+1} g_{i+1}^j | \eta_i^{1+j} |).}
The corresponding forcing term is

\[ f(x, t) = \frac{x^2(8-x)^{t-1}}{80(2-\alpha(x,t))} - (t+1)\left[ \frac{\Gamma(3)x^{2-\beta(x,t)}}{20\Gamma(3-\beta(x,t))} - \frac{\Gamma(4)x^{3-\beta(x,t)}}{160\Gamma(4-\beta(x,t))}\right], \]

Then Eq.(1) has the exact solution \( u(x, t) = \frac{(t+1)x^2(8-x)}{80}. \)

4. Numerical examples

Example 1. We take the various data, respectively, by

\[
\begin{align*}
\alpha(x,t) &= 0.5 + 0.01 \sin(5xt), \\
\beta(x,t) &= 1.5 + 0.01x^2t^2, \\
\kappa(x,t) &= -0.5 \cos(\beta(x,t)\pi/2), \\
\rho &= 1, \quad \sigma = 0, \quad (x, t) \in \Omega = (0, 8) \times (0, T].
\end{align*}
\]

The corresponding forcing term is

\[ f(x, t) = \frac{x^2(8-x)^{t-1}-\alpha(x,t)}{80(2-\alpha(x,t))} - (t+1)\left[ \frac{\Gamma(3)x^{2-\beta(x,t)}}{20\Gamma(3-\beta(x,t))} - \frac{\Gamma(4)x^{3-\beta(x,t)}}{160\Gamma(4-\beta(x,t))}\right]. \]
Table 1 gives the numerical solution, exact solution and absolute error at $T = 1$ of Example 1. Fig. 1 shows the solution behavior of Example 1 at $T = 0, T = 0.5$ and $T = 1$, respectively.

**Example 2.** In the example, we reselect the data, respectively, by

$$
\begin{align*}
\alpha(x, t) &= 1 - 0.8 e^{-xt}, \\
\beta(x, t) &= 1.7 + 0.1 e^{-\frac{x^2}{1000} - \frac{t}{50} - \frac{1}{\sigma}} , \\
\kappa(x, t) &= 1, \quad \rho = \sigma = \frac{1}{2}, \quad (x, t) \in \Omega = (0, 1) \times (0, T].
\end{align*}
$$

The corresponding forcing term is

$$
f(x, t) = 2x^2(1-x)^2\left[\frac{t^{2-\alpha(x,t)}}{\Gamma(3-\alpha(x,t))} + \frac{t^{2-\alpha(x,t)/2}}{\Gamma(3-\alpha(x,t)/2)} + \frac{\sec(\beta(x,t)\pi/2)}{2}(1+t^2)\right].$$

Then Eq. (1) has the exact solution $u(x, t) = (1 + t^2)x^2(1-x)^2$.

Table 2 gives the numerical solution, exact solution and absolute error at $T = 1$ of Example 2. Fig. 2 shows the solution behavior of Example 2 at $T = 0.25, T = 0.5, T = 0.75$, respectively. It can be seen that the numerical solution is in good agreement with the exact solution.

![Figure 1: The solution behavior of Example 1 at $T = 0, T = 0.5, T = 1$.](image1)

![Figure 2: The solution behavior of Example 2 at $T = 0.25, T = 0.5, T = 0.75$.](image2)

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