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# Preconditioned iterative methods for space-time fractional advection-diffusion equations

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## Abstract

In this paper, we propose practical numerical methods for solving a class of initial-boundary value problems of space-time fractional advection-diffusion equations. First, we propose an implicit method based on two-sided Grünwald formulae and discuss its stability and consistency. Then, we develop the preconditioned generalized minimal residual (preconditioned GMRES) method and preconditioned conjugate gradient normal residual (preconditioned CGNR) method with easily constructed preconditioners. Importantly, because resulting systems are Toeplitz-like, fast Fourier transform can be applied to significantly reduce the computational cost. We perform numerical experiments to demonstrate the efficiency of our preconditioners, even in cases with variable coefficients.

**Keywords:** Fractional diffusion equations; Toeplitz matrix; Preconditioner; Fast Fourier transform; Conjugate gradient normal residual method; Generalized minimal residual method.

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## 1. Introduction

In this study, we develop numerical approaches for solving the initial-boundary value problem of a space-time fractional advection-diffusion equation (STFDE) [1]:

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$$\begin{cases} \frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = -d_+(x,t)D_{a,x}^\beta u(x,t) - d_-(x,t)D_{x,b}^\beta u(x,t) + \\ \quad e_+(x,t)D_{a,x}^\gamma u(x,t) + e_-(x,t)D_{x,b}^\gamma u(x,t) + f(x,t), \\ u(x,0) = \phi(x), \quad a \leq x \leq b, \\ u(a,t) = u(b,t) = 0, \quad 0 < t \leq T, \end{cases} \quad (1)$$

where  $\alpha, \beta \in (0, 1]$ ,  $\gamma \in (1, 2]$ ,  $a < x < b$ , and  $0 < t \leq T$ . Here, parameters  $\alpha, \beta$  and  $\gamma$  are the order of STFDE,  $f(x, t)$  is the source term, and diffusion coefficient functions  $d_\pm(x, t)$  and  $e_\pm(x, t)$  are non-negative under the assumption that the flow is from left to right. STFDE can be regarded as a generalization of classical advection-diffusion equations with the first-order time derivative replaced by the Caputo fractional derivative of the order  $\alpha \in (0, 1]$  and the first- and second-order space derivatives replaced by the two-sided Riemann-Liouville fractional derivatives of orders  $\beta \in (0, 1]$  and  $\gamma \in (1, 2]$ , respectively. Namely, the time fractional derivative in Eq. (1) is the Caputo fractional derivative of order  $\alpha$  [2], which is denoted by

$$\frac{\partial^\alpha u(x,t)}{\partial t^\alpha} = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{\partial u(x,\psi)}{\partial \psi} \frac{d\psi}{(t-\psi)^\alpha}, \quad (2)$$

and the left-handed ( $D_{a,x}^\alpha$ ) and right-handed ( $D_{x,b}^\alpha$ ) space fractional derivatives in Eq. (1) are the Riemann-Liouville fractional derivatives of order  $\alpha$  [2, 3], which are defined by

$$D_{a,x}^\alpha u(x,t) = \frac{1}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_a^x \frac{u(s,t)}{(x-s)^{\alpha-m+1}} ds, \quad (3a)$$

and

$$D_{x,b}^\alpha u(x,t) = \frac{(-1)^m}{\Gamma(m-\alpha)} \frac{\partial^m}{\partial x^m} \int_x^b \frac{u(s,t)}{(s-x)^{\alpha-m+1}} ds, \quad (3b)$$

respectively, where  $\Gamma$  denotes the gamma function, and  $m$  is an integer satisfying  $m-1 \leq \alpha < m$ . In fact, when  $\alpha = \beta = 1$  and  $\gamma = 2$ , the above equation reduces to the classical advection-diffusion equation.

The study of fractional calculus can be traced back to late the 17th century [3–5], but it was not until the late 20th century that fractional differential equations (FDEs) became important because of their wide applications in the fields of finance [3, 6–8], physics [9–15], image processing [16], and biology [17]. Although analytical approaches such as the Fourier transform method, Laplace transform method, and Mellin transform method have been proposed to determine closed-form solutions [2], very few FDE analytical closed-form solutions are available. Therefore, research on numerical approximation and techniques for solving FDEs has attracted considerable interest (see [18–33] and the references therein). Importantly, traditional methods for solving FDEs tend to generate full coefficient matrices, which incur the computational cost  $\mathcal{O}(N^3)$  and storage  $\mathcal{O}(N^2)$ , with  $N$  being the number of grid points [27].

To optimize computational complexity, Meerschaet and Tadjeran [21, 22] proposed a shifted Grünwald discretization scheme with the property of unconditional stability. Later, Wang *et al.* [27] discovered that a linear system generated by this discretization has a special Toeplitz-like coefficient matrix; more precisely, this coefficient matrix can be expressed as a sum of diagonal-multiply-Toeplitz matrices. This implies that the storage requirement would be  $\mathcal{O}(N)$  rather than  $\mathcal{O}(N^2)$  and the complexity of the matrix-vector multiplication only requires  $\mathcal{O}(N \log N)$  operations by fast Fourier transform (FFT) [34–36]. Capitalizing

on this advantage, Wang *et al.* proposed the conjugate gradient normal residual (CGNR) method to solve a linear system, which has a computational cost of  $\mathcal{O}(N \log^2 N)$ , and numerical experiments show that the CGNR method is fast when diffusion coefficients are very small, i.e., discretized systems are well conditioned [37]. However, these systems become ill-conditioned when diffusion coefficients are not small. In this case, the CGNR method slowly converges. To overcome this limitation, preconditioning techniques have been introduced to improve the efficiency of the CG method with a total complexity of  $\mathcal{O}(N \log N)$  operations at each time step [38, 39]. For the same reason, we propose two preconditioned iterative methods, i.e., the preconditioned generalized minimal residual (GMRES) and CGNR methods, and observe the results related to the acceleration of the convergence of the iterative methods while solving Eq. (1).

This paper is organized as follows. In section 2, we propose an implicit difference method for Eq. (1) and prove that this scheme is unconditionally stable, convergent, and uniquely solvable. In section 3, we propose preconditioned GMRES method and CGNR methods for solving Eq. (1) by exploring the matrix representation of the implicit difference scheme. In section 4, we present the results of our numerical experiments, which demonstrate the efficiency of our numerical approaches. Finally, in section 5, we conclude our study.

## 2. Implicit difference method

In this section, we present an implicit difference method for solving Eq. (1) by discretizing STFDE defined by this equation. Unlike the approach reported by Liu *et al.* in [1], we use two-sided fractional derivatives to approximate the Riemann-Liouville derivatives in Eq. (3). We aim to demonstrate that when using two-sided fractional derivatives, this method is also unconditionally stable and convergent.

### 2.1. Discretization of STFDE

First, let  $m$  and  $n$  be two positive integers, and let  $h = (b - a)/m$  and  $\tau = T/n$  be the sizes of the time step and spatial grid, respectively. Then the spatial and temporal partitions can be defined by

$$x_i = a + ih, \quad i = 0, 1, \dots, m; \quad t_j = j\Delta t, \quad j = 0, 1, \dots, n,$$

and for convenience, henceforth we denote:

$$\begin{aligned} d_{+,i}^{(j)} &= d_+(x_i, t_j), \quad d_{-,i}^{(j)} = d_-(x_i, t_j), \quad e_{+,i}^{(j)} = e_+(x_i, t_j), \\ e_{-,i}^{(j)} &= e_-(x_i, t_j), \quad f_i^{(j)} = f(x_i, t_j), \quad \Delta_t u(x_i, t_j) = u(x_i, t_{j+1}) - u(x_i, t_j). \end{aligned}$$

Utilizing the forward difference formula, we know that the time fractional derivative for  $0 < \alpha < 1$  can be approximated by [1]:

$$\begin{aligned} \frac{\partial^\alpha u(x_i, t_{k+1})}{\partial t^\alpha} &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_{k+1}} \frac{\partial u(x_i, s)}{\partial s} \frac{ds}{(t_{k+1} - s)^\alpha} \\ &= \frac{1}{\Gamma(1-\alpha)} \sum_{j=0}^k \left( \left( \frac{1}{\tau} \Delta_t u(x_i, t_j) + \mathcal{O}(\tau) \right) \int_{t_j}^{t_{j+1}} (t_{k+1} - s)^{-\alpha} ds \right) + \mathcal{O}(\tau^{2-\alpha}) \\ &= \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{j=0}^k a_j \Delta_t u(x_i, t_{k-j}) + \mathcal{O}(\tau^{2-\alpha}), \end{aligned} \tag{4}$$

where  $a_j = (j+1)^{1-\alpha} - j^{1-\alpha}$ ,  $j = 0, 1, \dots, n$ . Also, the Riemann-Liouville derivatives in Eq. (3) can be approximated by adopting Grünwald estimates and shifted Grünwald estimates (see [21, Remark 2.5]) for parameters  $\beta$  and  $\gamma$ , respectively, i.e.,

$$D_{a,x}^{(\beta)} u(x_i, t_{k+1}) = \frac{1}{h^\beta} \sum_{j=0}^i g_j^{(\beta)} u(x_{i-j}, t_{k+1}) + \mathcal{O}(h), \quad (5a)$$

$$D_{x,b}^{(\beta)} u(x_i, t_{k+1}) = \frac{1}{h^\beta} \sum_{j=0}^{m-i} g_j^{(\beta)} u(x_{i+j}, t_{k+1}) + \mathcal{O}(h), \quad (5b)$$

$$D_{a,x}^{(\gamma)} u(x_i, t_{k+1}) = \frac{1}{h^\gamma} \sum_{j=0}^{i+1} g_j^{(\gamma)} u(x_{i-j+1}, t_{k+1}) + \mathcal{O}(h), \quad (5c)$$

$$D_{x,b}^{(\gamma)} u(x_i, t_{k+1}) = \frac{1}{h^\gamma} \sum_{j=0}^{i+1} g_j^{(\gamma)} u(x_{i+j-1}, t_{k+1}) + \mathcal{O}(h), \quad (5d)$$

where

$$\begin{aligned} g_0^{(\beta)} &= 1, \quad g_j^{(\beta)} = \frac{(-1)^j}{j!} \beta(\beta-1) \cdots (\beta-j+1), \quad j = 1, 2, \dots, \\ g_0^{(\gamma)} &= 1, \quad g_j^{(\gamma)} = \frac{(-1)^j}{j!} \gamma(\gamma-1) \cdots (\gamma-j+1), \quad j = 1, 2, \dots \end{aligned}$$

Let

$$\omega_1 = \frac{\Gamma(2-\alpha)\tau^\alpha}{h^\beta}, \quad \omega_2 = \frac{\Gamma(2-\alpha)\tau^\alpha}{h^\gamma}, \quad \omega_3 = \Gamma(2-\alpha)\tau^\alpha,$$

and  $u_i^{(j)}$  represent the numerical approximation of  $u(x_i, t_j)$ . Using Eqs. (4) and (5), we see that the solution for Eq. (1) can be approximated by the following *implicit difference method*:

$$\begin{aligned} u_i^{(k+1)} + \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=0}^i g_j^{(\beta)} u_{i-j}^{(k+1)} + d_{-,i}^{(k+1)} \sum_{j=0}^{m-i} g_j^{(\beta)} u_{i+j}^{(k+1)} \right) - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} u_{i-j+1}^{(k+1)} \right. \\ \left. + e_{-,i}^{(k+1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} u_{i+j-1}^{(k+1)} \right) = u_i^{(k)} - \sum_{j=1}^k a_j (u_i^{(k-j+1)} - u_i^{(k-j)}) + \omega_3 f_i^{(k+1)}, \end{aligned} \quad (6)$$

where  $i = 1, \dots, m-1$ ;  $k = 0, \dots, n-1$ , and the boundary and initial conditions can be discretized as follows:

$$u_i^{(0)} = \phi(x_i), \quad i = 0, \dots, m; \quad u_0^{(k)} = u_m^{(k)} = 0, \quad k = 1, \dots, n.$$

## 2.2. Analysis of the implicit difference method

To analyze the stability and convergence of the implicit difference method given above, we first let  $U_i^{(k)}$  be the approximation solution of  $u_i^{(k)}$  in the method given by Eq. (6), and let  $\xi_i^{(k)} = U_i^{(k)} - u_i^{(k)}$ ,  $i = 1, \dots, m-1$ ;  $k = 0, \dots, n-1$ , be the error satisfying the equation

$$\begin{aligned} \xi_i^{(k+1)} + \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=0}^i g_j^{(\beta)} \xi_{i-j}^{(k+1)} + d_{-,i}^{(k+1)} \sum_{j=0}^{m-i} g_j^{(\beta)} \xi_{i+j}^{(k+1)} \right) - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} \xi_{i-j+1}^{(k+1)} \right. \\ \left. + e_{-,i}^{(k+1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} \xi_{i+j-1}^{(k+1)} \right) = \xi_i^{(k)} - \sum_{j=1}^k a_j (\xi_i^{(k-j+1)} - \xi_i^{(k-j)}). \end{aligned} \quad (7)$$

Correspondingly, we assume  $E^{(k+1)} = [\xi_1^{(k)}, \xi_2^{(k)}, \dots, \xi_{m-1}^{(k)}]^\top$ ,  $k = 0, \dots, n-1$ . It is obvious upon inspection that the method given by Eq. (6) is stable, once we can show that

$$\|E^{(k+1)}\|_\infty \leq \|E^{(0)}\|_\infty.$$

To achieve this purpose, the following results given in [21, 22, 27] are required.

**Lemma 2.1.** *The coefficients  $a_j$ ,  $g_j^{(\beta)}$ ,  $g_j^{(\gamma)}$ , for  $j = 1, 2, \dots$ , satisfy:*

1.  $1 = a_0 > a_1 > a_2 > \dots > a_j \rightarrow 0$ , as  $j \rightarrow \infty$ ,
2.  $g_0^{(\beta)} = 1$ ,  $g_j^{(\beta)} < 0$ , for  $j = 1, 2, \dots$ , and  $\sum_{j=0}^\infty g_j^{(\beta)} = 0$ ,
3.  $g_1^{(\gamma)} = -\gamma < 0$ ,  $g_j^{(\gamma)} > 0$ , for  $j \neq 1$ , and  $\sum_{j=0}^\infty g_j^{(\gamma)} = 0$ .
4.  $g_j^{(\beta)} = \mathcal{O}(j^{-(\beta+1)})$  and  $g_j^{(\gamma)} = \mathcal{O}(j^{-(\gamma+1)})$ .

We note that Lemma 2.1 implies that

$$\sum_{j=0}^k g_j^{(\beta)} > 0 \text{ and } \sum_{j=0}^{k+1} g_j^{(\gamma)} < 0, \quad \text{for } k = 0, 1, \dots$$

This observation can also confirm the stability of the method given by Eq. (6).

**Theorem 2.2.** *The implicit difference method given by Eq. (6) for the time-space fractional diffusion equation is unconditionally stable, i.e.,:*

$$\|E^{(k+1)}\|_\infty \leq \|E^{(0)}\|_\infty, \quad 0 \leq k \leq n-1. \quad (8)$$

**Proof:** First, without loss of generality, we may assume that, in our proof, the diffusion coefficient functions  $d_+(x, t) = d_+$ ,  $d_-(x, t) = d_-$ ,  $e_+(x, t) = e_+$  and  $e_-(x, t) = e_-$  are constants. Suppose that  $k = 0$ , and let  $\xi_\ell^{(1)} = \|E^{(1)}\|_\infty := \max_{1 \leq i \leq m-1} |\xi_i^{(1)}|$ . Then

$$\begin{aligned} |\xi_\ell^{(1)}| &\leq \left[ 1 + \omega_1 \left( d_{+, \ell}^{(k+1)} \sum_{j=0}^\ell g_j^{(\beta)} + d_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \right) - \omega_2 \left( e_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} + e_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \right) \right] |\xi_\ell^{(1)}| \\ &\leq |\xi_\ell^{(1)}| + \omega_1 \left( d_{+, \ell}^{(1)} \sum_{j=0}^\ell g_j^{(\beta)} |\xi_{\ell-j}^{(1)}| + d_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} |\xi_{\ell+j}^{(1)}| \right) - \omega_2 \left( e_{+, \ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} |\xi_{\ell-j+1}^{(1)}| + e_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} |\xi_{\ell+j-1}^{(1)}| \right) \\ &\leq \left| \xi_\ell^{(1)} + \omega_1 \left( d_{+, \ell}^{(1)} \sum_{j=0}^\ell g_j^{(\beta)} \xi_{\ell-j}^{(1)} + d_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \xi_{\ell+j}^{(1)} \right) - \omega_2 \left( e_{+, \ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \xi_{\ell-j+1}^{(1)} + e_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \xi_{\ell+j-1}^{(1)} \right) \right| \\ &= |\xi_\ell^{(0)}| \leq \|E^{(0)}\|_\infty. \end{aligned}$$

Here, the second and third inequalities are true due to the fact given in Lemma 2.1 and to the triangle inequality of absolute value. Now suppose that for some integer  $k \geq 0$ , the result is established, i.e.,:

$$\|E^{(j)}\|_\infty \leq \|E^{(0)}\|_\infty, \quad \text{for } j \leq k.$$

As we did earlier for  $k = 0$ , let  $\xi_\ell^{(k+1)} = \max_{1 \leq i \leq m-1} |\xi_i^{(k+1)}|$ . By Lemma 2.1, we can see that

$$\begin{aligned}
 |\xi_\ell^{(k+1)}| &\leq \left| \xi_\ell^{(k+1)} + \omega_1 \left( d_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \xi_{\ell-j}^{(k+1)} + d_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \xi_{\ell+j}^{(k+1)} \right) \right. \\
 &\quad \left. - \omega_2 \left( e_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \xi_{\ell-j+1}^{(k+1)} + e_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \xi_{\ell+j-1}^{(k+1)} \right) \right| \\
 &= \left| \xi_\ell^k - \sum_{j=1}^k a_j (\xi_\ell^{k-j+1} - \xi_\ell^{k-j}) \right| = \left| \sum_{j=1}^k (a_{j-1} - a_j) \xi_\ell^{(k-j+1)} + a_k \xi_\ell^{(0)} \right| \\
 &\leq \|E^{(0)}\|_\infty.
 \end{aligned}$$

The preceding result, which follows from the assumption that the coefficient functions are constant, does not provide complete results. In fact, we can see that the above proof requires only properties of the non-negativity of the coefficient functions. Thus, the result for non-constant coefficient functions can be proved similarly.  $\square$

Our next theorem analyzes the convergence of the implicit method given in Eq. (6). To this end, recall that  $u(x_i, t_j)$ ,  $i = 1, \dots, n-1$ ;  $j = 0, \dots, n-1$ , denotes the exact solution of Eq. (1) at mesh point  $(x_i, t_j)$  and  $u_i^{(j)}$ ,  $i = 1, \dots, n-1$ ;  $j = 0, \dots, n-1$ , represents the solution of the method given by Eq. (6). Let us assume that  $\psi_i^{(k)} = u(x_i, t_k) - u_i^{(k)}$  and  $\Psi^{(k)} = (\psi_1^{(k)}, \psi_2^{(k)}, \dots, \psi_{m-1}^{(k)})^\top$ . Note that, by construction,  $\Psi^{(0)} = \mathbf{0}$ , since  $u_i^{(0)} = \psi(x_i) = u(x_i, 0)$ ,  $i = 1, \dots, m-1$ .

Using this notation, we consider

$$\begin{cases} \psi_i^{(1)} + \omega_1 \left( d_{+, i}^{(1)} \sum_{j=0}^i g_j^{(\beta)} \psi_{i-j}^{(1)} + d_{-, i}^{(1)} \sum_{j=0}^{m-i} g_j^{(\beta)} \psi_{i+j}^{(1)} \right) - \omega_2 \left( e_{+, i}^{(1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} \psi_{i-j+1}^{(1)} \right. \\ \quad \left. + e_{-, i}^{(1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} \psi_{i+j-1}^{(1)} \right) = R_i^{(1)}, \\ \psi_i^{(k+1)} + \omega_1 \left( d_{+, i}^{(k+1)} \sum_{j=0}^i g_j^{(\beta)} \psi_{i-j}^{(k+1)} + d_{-, i}^{(k+1)} \sum_{j=0}^{m-i} g_j^{(\beta)} \psi_{i+j}^{(k+1)} \right) - \omega_2 \left( e_{+, i}^{(k+1)} \sum_{j=0}^{i+1} g_j^{(\gamma)} \right. \\ \quad \left. \psi_{i-j+1}^{(k+1)} + e_{-, i}^{(k+1)} \sum_{j=0}^{m-i+1} g_j^{(\gamma)} \psi_{i+j-1}^{(k+1)} \right) = \psi_i^{(k)} - \sum_{j=1}^k a_j (\psi_i^{(k-j+1)} - \psi_i^{(k-j)}) + R_i^{(k+1)}, \\ 1 \leq i \leq m-1, 1 \leq k \leq n-1. \end{cases} \quad (9)$$

In this way, we can observe from Eqs. (4) and (5) that:

$$R_i^{(k+1)} = \mathcal{O}((\tau^2 + \tau^\alpha h)), \quad 1 \leq i \leq m-1; 0 \leq k \leq n-1. \quad (10)$$

Thus, a way suffices to do the convergence analysis by generating an upper bound of  $\|\Psi^{(k+1)}\|_\infty$ ,  $k = 0, 1, \dots, n-1$ , as follows:

**Theorem 2.3.**

$$\|\Psi^{(k+1)}\|_\infty \leq C a_k^{-1} (\tau^2 + \tau^\alpha h), \quad k = 0, \dots, n-1, \quad (11)$$

for some constant  $C$ .

**Proof:** Corresponding to Eq. (10), we assume for convenience that there is a positive constant  $C$  such that:

$$|R_i^{(k+1)}| \leq C(\tau^2 + \tau^\alpha h), \quad 1 \leq i \leq m-1; 0 \leq k \leq n-1.$$

Then, the poof is by mathematical induction on  $k$ . Let  $|\psi_\ell^1| = \|\Psi^1\|_\infty := \max_{1 \leq i \leq m-1} |\psi_i^1|$ . Observe from Eq. (9) that if  $k = 0$ , then we have:

$$\begin{aligned} |\psi_\ell^{(1)}| &\leq \left[ 1 + \omega_1 \left( d_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} + d_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \right) - \omega_2 \left( e_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} + e_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \right) \right] |\psi_\ell^{(1)}| \\ &\leq |\psi_\ell^{(1)}| + \omega_1 \left( d_{+, \ell}^{(1)} \sum_{j=0}^{\ell} g_j^{(\beta)} |\psi_{\ell-j}^{(1)}| + d_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} |\psi_{\ell+j}^{(1)}| \right) - \omega_2 \left( e_{+, \ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} |\psi_{\ell-j+1}^{(1)}| + e_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} |\psi_{\ell+j-1}^{(1)}| \right) \\ &\leq \left| \psi_\ell^{(1)} + \omega_1 \left( d_{+, \ell}^{(1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \psi_{\ell-j}^{(1)} + d_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \psi_{\ell+j}^{(1)} \right) - \omega_2 \left( e_{+, \ell}^{(1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \psi_{\ell-j+1}^{(1)} + e_{-, \ell}^{(1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \psi_{\ell+j-1}^{(1)} \right) \right| \\ &= |R_\ell^{(1)}| \leq C a_0^{-1} (\tau^2 + \tau^\alpha h), \end{aligned}$$

namely,

$$\|\Psi^1\|_\infty \leq C a_0^{-1} (\tau^2 + \tau^\alpha h),$$

Suppose that the result is valid for some integer  $k \geq 0$ , i.e.,:

$$\|\Psi^j\|_\infty \leq C a_{k-1}^{-1} (\tau^2 + \tau^\alpha h), \quad j = 1, \dots, k-1. \quad (12)$$

Let  $|\psi_\ell^{k+1}| = \|\Psi^{k+1}\|_\infty := \max_{1 \leq i \leq m-1} |\psi_i^{k+1}|$ . It follows that

$$\begin{aligned} |\psi_\ell^{k+1}| &\leq \left| \psi_\ell^{(k+1)} + \omega_1 \left( d_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell} g_j^{(\beta)} \psi_{\ell-j}^{(k+1)} + d_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell} g_j^{(\beta)} \psi_{\ell+j}^{(k+1)} \right) \right. \\ &\quad \left. - \omega_2 \left( e_{+, \ell}^{(k+1)} \sum_{j=0}^{\ell+1} g_j^{(\gamma)} \psi_{\ell-j+1}^{(k+1)} + e_{-, \ell}^{(k+1)} \sum_{j=0}^{m-\ell+1} g_j^{(\gamma)} \psi_{\ell+j-1}^{(k+1)} \right) \right| \\ &= \left| \psi_\ell^k - \sum_{j=1}^k a_j (\psi_\ell^{k-j+1} - \psi_\ell^{k-j}) \right| = \left| \sum_{j=1}^k (a_{j-1} - a_j) \psi_\ell^{(k-j+1)} + a_k \psi_\ell^{(0)} + R_\ell^{(k+1)} \right| \\ &\leq \sum_{j=1}^k (a_{j-1} - a_j) |\psi_\ell^{(k-j+1)}| + |R_\ell^{(k+1)}| \\ &\leq C \left( a_k + \sum_{j=1}^k (a_{j-1} - a_j) \right) a_k^{-1} (\tau^2 + \tau^\alpha h) \leq C a_k^{-1} (\tau^2 + \tau^\alpha h), \end{aligned}$$

since  $a_{j-1} - a_j > 0$ ,  $j = 1, \dots, k$ , and  $\psi_\ell^{(0)} = 0$ . □

It was shown in [1] that:

$$\lim_{k \rightarrow \infty} \frac{a_k^{-1}}{k^\alpha} = \frac{1}{1 - \alpha}. \quad (13)$$

By Eqs. (11)) and (13), we immediately have the following result, which demonstrates the convergence of our implicit method.



**Corollary 2.4.** Let  $u_i^{(k)}$ ,  $i = 1, \dots, m-1$ ;  $k = 1, \dots, n$  be the numerical solution computed by the implicit difference method given by Eq. (6). Then, there exists a constant  $C$  such that:

$$|u(x_i, t_k) - u_i^{(k)}| \leq C(\tau^{2-\alpha} + h), \quad i = 1, \dots, m-1; k = 1, \dots, n. \quad (14)$$

We note that the above approach used to analyze stability and convergence is simply a follow-up to that used by Liu *et al.* in [1]. Our focus in this work is to apply the efficient CGNR and GMRES methods to solve the linear system arising from the method given by Eq. (6) with respect to suitably constructed preconditioners.

### 3. Preconditioned iterative methods

Before investigating preconditioning techniques, the matrix representation of Eq. (6) must first be elaborated upon. To facilitate our discussion, we use  $I_{m-1}$  to denote the identity matrix of order  $m-1$ . For  $1 \leq j \leq n-1$ , let:

$$\begin{aligned} \mathbf{u}^{(j)} &= [u_1^{(j)}, u_2^{(j)}, \dots, u_{m-1}^{(j)}]^\top, \quad \mathbf{f}^{(j)} = [f_1^{(j)}, f_2^{(j)}, \dots, f_{m-1}^{(j)}]^\top, \\ D_+^{(j)} &= \text{diag}(d_{+,1}^{(j)}, \dots, d_{+,m-1}^{(j)}), \quad D_-^{(j)} = \text{diag}(d_{-,1}^{(j)}, \dots, d_{-,m-1}^{(j)}), \\ E_+^{(j)} &= \text{diag}(e_{+,1}^{(j)}, \dots, e_{+,m-1}^{(j)}), \quad E_-^{(j)} = \text{diag}(e_{-,1}^{(j)}, \dots, e_{-,m-1}^{(j)}), \end{aligned}$$

and  $\mathbf{u}^{(0)} = (\phi_1^{(0)}, \phi_2^{(0)}, \dots, \phi_{m-1}^{(0)})^\top$ . Let  $G_\beta$  and  $G_\gamma$  be two Toeplitz matrices defined by

$$G_\beta = \begin{bmatrix} g_0^{(\beta)} & 0 & \cdots & \cdots & 0 \\ g_1^{(\beta)} & g_0^{(\beta)} & 0 & \cdots & 0 \\ \vdots & g_1^{(\beta)} & g_0^{(\beta)} & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ g_{m-2}^{(\beta)} & \ddots & \ddots & \ddots & g_0^{(\beta)} \end{bmatrix}, \quad G_\gamma = \begin{bmatrix} g_1^{(\gamma)} & g_0^{(\gamma)} & 0 & \cdots & 0 & 0 \\ g_2^{(\gamma)} & g_1^{(\gamma)} & g_0^{(\gamma)} & 0 & \cdots & 0 \\ \vdots & g_2^{(\gamma)} & g_1^{(\gamma)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{m-2}^{(\gamma)} & \ddots & \ddots & \ddots & g_1^{(\gamma)} & g_0^{(\gamma)} \\ g_{m-1}^{(\gamma)} & g_{m-2}^{(\gamma)} & \cdots & \cdots & g_2^{(\gamma)} & g_1^{(\gamma)} \end{bmatrix}.$$

Upon substitution, we see that method given by Eq. (6) is equivalent to a matrix equation with the form:

$$(I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)} = \mathbf{b}^{(k+1)}, \quad (15)$$

where

$$\mathbf{b}^{(k+1)} = \sum_{j=1}^k (a_{k-j} - a_{k-j+1})\mathbf{u}^{(j)} + a_k \mathbf{u}^{(0)} + \omega_3 \mathbf{f}^{k+1}$$

and

$$A^{(k+1)} = \omega_1 (D_+^{(k+1)} G_\beta + D_-^{(k+1)} G_\beta^\top) - \omega_2 (E_+^{(k+1)} G_\gamma + E_-^{(k+1)} G_\gamma^\top). \quad (16)$$

Now we can define the corresponding matrix equation of the method given by Eq. (6). An intuitive question might be to ask whether the matrix equation is uniquely solvable. Before answering, we make an interesting observation regarding the following result.

**Theorem 3.1.** *The matrix  $I_{m-1} + A^{(k+1)}$  in Eq. (15) is a nonsingular, strictly diagonally dominant  $M$ -matrix.*

**Proof:** Let  $a_{ij}^{(k+1)}$  be the  $(i, j)$  entry of the matrix  $A^{(k+1)}$  in Eq. (15). Note that we have from Eq. (15):

$$\begin{aligned}
 & a_{ii}^{(k+1)} - \sum_{j=1, j \neq i}^{m-1} |a_{ij}^{(k+1)}| \\
 &= \omega_1 \left( d_{+,i}^{(k+1)} + d_{-,i}^{(k+1)} \right) g_0^{(\beta)} - \omega_1 \left( d_{+,i}^{(k+1)} \sum_{j=1}^{i-1} g_j^{(\beta)} + d_{-,i}^{(k+1)} \sum_{j=1}^{m-i-1} g_j^{(\beta)} \right) \\
 & \quad - \omega_2 \left( e_{+,i}^{(k+1)} + e_{-,i}^{(k+1)} \right) g_1^{(\gamma)} - \omega_2 \left( e_{+,i}^{(k+1)} \sum_{j=0, j \neq 1}^i g_j^{(\gamma)} + e_{-,i}^{(k+1)} \sum_{j=0, j \neq 1}^{m-i} g_j^{(\gamma)} \right) \\
 & \geq \omega_1 \left( d_{+,i}^{(k+1)} + d_{-,i}^{(k+1)} \right) g_0^{(\beta)} - \omega_1 \left( d_{+,i}^{(k+1)} + d_{-,i}^{(k+1)} \right) \sum_{j=1}^{\infty} g_j^{(\beta)} \\
 & \quad - \omega_2 \left( e_{+,i}^{(k+1)} + e_{-,i}^{(k+1)} \right) g_1^{(\gamma)} - \omega_2 \left( e_{+,i}^{(k+1)} + e_{-,i}^{(k+1)} \right) \sum_{j=0, j \neq 1}^{\infty} g_j^{(\gamma)} = 0.
 \end{aligned} \tag{17}$$

At first glance, this implies that the coefficient matrix  $I_{m-1} + A^{(k+1)}$  is strictly diagonally dominant and  $(I_{m-1} + A^{(k+1)})\mathbf{1} > 0$ , where  $\mathbf{1}$  is a vector of length  $n-1$  with all entries equal to one. We observe further that  $a_{i,j} \leq 0$ , for all  $i \neq j$ , i.e., the matrix  $I_{m-1} + A^{(k+1)}$  is a  $Z$ -matrix. This completes the proof.  $\square$

With the aid of Theorem 3.1, we quickly point out that the solution of Eq. (15) is unique. More significantly, since Eq. (15) is a matrix representation of the method given by Eq. (6), we then obtain the following result.

**Corollary 3.2.** *The difference method given by Eq. (6) is uniquely solvable.*

We have completed the proof of the unique solvability of the implicit difference scheme given in Eq. (6), and we are now ready to apply the popular and effective iterative CGNR and GMRES methods to solve Eq. (15). In section 4, we will see that when solving large-scale equations the systems would become nearly singular and ill-conditioned. For such problems, we apply the preconditioning technique to accelerate the iterative process.

To achieve this purpose, we start by decomposing matrices  $G_\beta$  and  $G_\gamma$  as

$$\begin{aligned}
 G_\beta &= G_{\beta,\ell} + (G_\beta - G_{\beta,\ell}), \\
 G_\gamma &= G_{\gamma,\ell} + (G_\gamma - G_{\gamma,\ell}),
 \end{aligned}$$

where

$$\begin{aligned}
 G_{\beta,\ell} &= \begin{bmatrix} g_0^{(\beta)} & & & & \\ \vdots & g_0^{(\beta)} & & & \\ g_{\ell-1}^{(\beta)} & & \ddots & & \\ & \ddots & & \ddots & \\ & & g_{\ell-1}^{(\beta)} & \cdots & g_0^{(\alpha)} \end{bmatrix} + \begin{bmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & g_{\ell}^{(\beta)} & \\ & & & & \ddots \\ & & & & & \sum_{j=\ell}^{m-2} g_j^{(\beta)} \end{bmatrix}, \\
 G_{\gamma,\ell} &= \begin{bmatrix} g_1^{(\gamma)} & g_0^{(\gamma)} & & & \\ \vdots & g_1^{(\gamma)} & g_0^{(\gamma)} & & \\ g_{\ell}^{(\gamma)} & & \ddots & \ddots & \\ & \ddots & & \ddots & g_0^{(\alpha)} \\ & & g_{\ell}^{(\gamma)} & \cdots & g_1^{(\gamma)} \end{bmatrix} + \begin{bmatrix} 0 & & & & \\ & \ddots & & & \\ & & 0 & & \\ & & & g_{\ell+1}^{(\gamma)} & \\ & & & & \ddots \\ & & & & & \sum_{j=\ell+1}^{m-1} g_j^{(\gamma)} \end{bmatrix}.
 \end{aligned}$$

Namely, the matrix  $A^{(k+1)}$  can be decomposed as

$$A^{(k+1)} = A_{\ell}^{(k+1)} + B_{\ell}^{(k+1)},$$

where

$$\begin{aligned}
 A_{\ell}^{(k+1)} &= \omega_1(D_+^{k+1}G_{\beta,\ell} + D_-^{k+1}G_{\beta,\ell}^{\top}) - \omega_2(E_+^{k+1}G_{\gamma,\ell} + E_-^{k+1}G_{\gamma,\ell}^{\top}), \\
 B_{\ell}^{(k+1)} &= A^{(k+1)} - A_{\ell}^{(k+1)}.
 \end{aligned}$$

Note from Lemma 2.1 that it is easy to show that the Toeplitz matrices  $G_{\beta}$  and  $-G_{\gamma}$  are  $M$ -matrices and strictly diagonally dominant. Therefore, this implies that the matrices  $G_{\beta,\ell}$  and  $G_{\gamma,\ell}$  are strictly diagonally dominant  $M$ -matrices, since the matrices  $G_{\beta,\ell}$  and  $G_{\gamma,\ell}$  have the same row sums as  $G_{\beta}$  and  $G_{\gamma}$ , respectively. In this way, the following fact can be directly realized.

**Theorem 3.3.** *The matrix  $I_{m-1} + A_{\ell}^{(k+1)}$  is a nonsingular, strictly diagonally dominant  $M$ -matrix for all  $\ell$ .*

In addition, Lemma 2.1 implies that:

$$\begin{aligned}
 &\frac{\|(I_{m-1} + A^{(k+1)}) - (I_{m-1} + A_{\ell}^{(k+1)})\|_{\infty}}{\|I_{m-1} - A^{(k+1)}\|_{\infty}} \\
 &\leq \frac{\frac{1}{h^{\gamma}}\|(D_+^{k+1}(G_{\beta} - G_{\beta,\ell}) + D_-^{k+1}(G_{\beta} - G_{\beta,\ell})^{\top}) - (E_+^{k+1}(G_{\gamma} - G_{\gamma,\ell}) + E_-^{k+1}(G_{\gamma} - G_{\gamma,\ell})^{\top})\|_{\infty}}{\frac{1}{h^{\beta}}\|(D_+^{(k+1)}G_{\beta} + D_-^{(k+1)}G_{\beta}^{\top}) - (E_+^{(k+1)}G_{\gamma} + E_-^{(k+1)}G_{\gamma}^{\top})\|_{\infty}} \\
 &= O(k^{-\beta}),
 \end{aligned}$$

since  $\|G_{\beta} - G_{\beta,\ell}\|_{\infty} = O(k^{-\beta})$ ,  $\|G_{\gamma} - G_{\gamma,\ell}\|_{\infty} = O(k^{-\gamma})$ , and  $h = (b-a)/m$  [39]. In other words, the relative difference between  $I_{m-1} + A^{(k+1)}$  and  $I_{m-1} + A_{\ell}^{(k+1)}$  can become very small as  $k$  becomes

large enough. Observe further that the banded matrix  $I_{m-1} + A_\ell^{(k+1)}$  is a sparse matrix consisting of  $2\ell - 1$  nonzero diagonal entries. With this in hand, an efficient preconditioner for the linear system (15) is attainable by simply choosing  $I_{m-1} + A_\ell^{(k+1)}$ . We assume here that the reader is familiar with the fundamental terminology and iterative approaches of the preconditioned GMRES and CGNR methods. For a comprehensive explanation of these iterative techniques, the reader is referred to monograph [40] written by Saad.

### 3.1. Preconditioned GMRES method

The GMRES method, proposed in 1986 in [41], is one of the most popular and effective methods for solving nonsymmetric linear systems. However, for large sparse systems, the application of preconditioning techniques can reduce the number of conditions, and hence improve the convergence rate. Let  $P_\ell^{(k+1)} := I_{m-1} + A_\ell^{(k+1)}$ . Our purpose here is to replace the linear system of Eq. (15) with the preconditioned linear system:

$$(P_\ell^{(k+1)})^{-1}(I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)} = (P_\ell^{(k+1)})^{-1}\mathbf{b}^{(k+1)} \quad (18)$$

and generate the same solution. We then solve Eq. (18) with respect to the left-preconditioned GMRES method proposed in [39]. To make this work more self-contained, we quote this method as follows:

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#### Preconditioned GMRES( $\rho$ ) method

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At each time step  $t^{(k+1)}$ , we choose  $\mathbf{u}_0$  as initial guess for  $\mathbf{u}^{(k+1)}$   
 Set  $\mu := 0$ , and compute the LU factorization:  $P_\ell^{(k+1)} = LU$   
 Compute  $\mathbf{r} := \mathbf{b}^{(k+1)} - (I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)}$ , and assign  $\mathbf{r}_t := \mathbf{r}$   
 While  $\mu \leq \text{IterMax}$  and  $\|\mathbf{r}_t\|_2 / \|\mathbf{b}^{(k+1)}\|_2 > \epsilon$  do  
      $\mu := \mu + 1$   
     Compute  $\mathbf{r}_w := U^{-1}L^{-1}\mathbf{r}$ ,  $\beta := \|\mathbf{r}_w\|$ ,  $\mathbf{v}_1 := \mathbf{r}_w / \beta$   
     Assign  $j := 0$  and  $V_1 := \mathbf{v}_1$   
     While  $j \leq \rho$  and  $\|\mathbf{r}_t\|_2 / \|\mathbf{b}^{(k+1)}\|_2 > \epsilon$  do  
          $j := j + 1$   
         Compute  $\mathbf{w} := U^{-1}L^{-1}(I_{m-1} + A^{(k+1)})\mathbf{v}_j$   
         For  $i = 1, \dots, j$  do  
              $h_{i,j} = \mathbf{v}_i^T * \mathbf{w}$   
              $\mathbf{w} := \mathbf{w} - h_{i,j}\mathbf{v}_i$   
         Enddo  
         Compute  $h_{j+1,j} = \|\mathbf{w}\|_2$  and  $\mathbf{v}_{j+1} := \mathbf{w} / h_{j+1,j}$   
         Assign  $V_{j+1} := [V_j, \mathbf{v}_{j+1}]$  and  $H_j := [h_{\gamma,\delta}]_{1 \leq \gamma \leq j+1, 1 \leq \delta \leq j}$   
         Compute  $\mathbf{y}_j := \text{argmin}_{\mathbf{y}} \|\beta \mathbf{e}_1 - H_j \mathbf{y}\|_2$   
         Compute the residual  $\mathbf{r}_t := \mathbf{r} - LU V_{j+1} H_j \mathbf{y}_j$   
     Enddo  
      $\mathbf{r} := \mathbf{r}_t$   
      $\mathbf{u}^{(k+1)} := \mathbf{u}^{(k+1)} + V_j \mathbf{y}_j$   
 Enddo

Here,  $IterMax$  denotes the maximal number of iterations,  $\epsilon$  denotes the given relative accuracy of the residual,  $\rho$  denotes that the GMRES method is restarted after  $\rho$  iterations, and the symbols  $\mathbf{r}_t$  and  $\mathbf{r}_w$  represent the current residual of the original linear system in Eq. (15) and that of the preconditioned linear system in Eq. (18), respectively. Associated with this preconditioned method are two major aspects of the computational work:

- the computation of  $\mathbf{w} = U^{-1}L^{-1}(I_{m-1} + A^{(k+1)})\mathbf{v}_j$  and
- the computation of  $\mathbf{r}_t = \mathbf{r} - LUV_{j+1}H_j\mathbf{y}_j$ .

We observe from (16) that

$$A^{(k+1)}\mathbf{v} = \omega_1(D_+^{(k+1)}G_\beta\mathbf{v} + D_-^{(k+1)}G_\beta^\top\mathbf{v}) - \omega_2(E_+^{(k+1)}G_\gamma\mathbf{v} + E_-^{(k+1)}G_\gamma^\top\mathbf{v}),$$

where  $G_\gamma$  and  $G_\beta$  are two  $(m-1)$ -by- $(m-1)$  Toeplitz matrices and can be stored only with  $m-1$  and  $m$  entries, respectively. This implies that the major work of computing  $A^{(k+1)}\mathbf{v}$  includes four Toeplitz matrix-vector multiplications,  $G_\beta\mathbf{v}$ ,  $G_\beta^\top\mathbf{v}$ ,  $G_\gamma\mathbf{v}$  and  $G_\gamma^\top\mathbf{v}$ , which can be obtained using FFT with only  $\mathcal{O}((m-1)\log(m-1))$  operations [34, 36, 42]. It might be important to note that, based on the specific structure of the matrix  $G_s$ , where  $s = \beta$  or  $\gamma$ , the calculations of  $G_s\mathbf{v}$  and  $G_s^\top\mathbf{v}$  can be performed simultaneously, by computing  $G_s(\mathbf{v} + \sqrt{-1}\hat{\mathbf{v}})$ , where  $\hat{\mathbf{v}} = (v_{m-1}, v_{m-2}, \dots, v_1)^\top$ .

Since the matrix  $P_\ell^{(k+1)}$  is banded and strongly diagonally dominant,  $P_\ell^{(k+1)}$  admits a banded  $LU$  factorization [43, Proposition 2.3], i.e.,:

$$P_\ell^{(k+1)} = LU, \quad (19)$$

where  $L$  and  $U$  are banded with bandwidth  $\ell$  and can be obtained in about  $\mathcal{O}((m-1)\ell^2)$  operations when  $\ell$  is small compared to  $m-1$ . This implies that given a vector  $\mathbf{x}$  of an appropriate size, the matrix-vector multiplications  $L\mathbf{x}$ ,  $U\mathbf{x}$ ,  $L^{-1}\mathbf{x}$ , and  $U^{-1}\mathbf{x}$  require only  $\mathcal{O}((m-1)\ell)$  operations. Thus, the computation of the vector  $\mathbf{w}$  requires  $\mathcal{O}((m-1)\log(m-1))$  operations, and the computation of the vector  $\mathbf{r}_t$  requires  $\mathcal{O}((m-1)(j+\ell))$  operations since  $V_{j+1}$  and  $H_j$  are matrices of sizes  $(m-1)$ -by- $(j+1)$  and  $(j+1)$ -by- $j$ .

### 3.2. Preconditioned CGNR method

To solve the nonsymmetric linear system in Eq. (15), one might consider the application of the conjugate gradient (CG) method to the normal equation

$$(I_{m-1} + A^{(k+1)})^\top(I_{m-1} + A^{(k+1)})\mathbf{u}^{(k+1)} = (I_{m-1} + A^{(k+1)})^\top\mathbf{b}^{(k+1)}. \quad (20)$$

This approach is known as the CGNR method. One disadvantage of applying the CG method directly to Eq. (20) is that the condition number of  $(I_{m-1} + A^{(k+1)})^\top(I_{m-1} + A^{(k+1)})$  is the square of that of  $I_{m-1} + A^{(k+1)}$ . Thus, the convergence process of the CGNR method would be very slow. To accelerate the entire process, we choose  $(P_\ell^{(k+1)})^\top P_\ell^{(k+1)}$  as the preconditioner for the normal Eq. (20).

Note that the main computational work in the preconditioned CGNR method has two parts [40]. One is the matrix-vector multiplication  $(I_{m-1} + A^{(k+1)})^\top(I_{m-1} + A^{(k+1)})\mathbf{v}$  for some vector  $\mathbf{v}$ . The other is the calculation of the solution of the linear system  $(P_\ell^{(k+1)})^\top P_\ell^{(k+1)}\mathbf{w} = \mathbf{z}$  for some vectors  $\mathbf{w}$  and  $\mathbf{z}$ . Of course, like the preconditioned GMRES method, the calculation of the matrix-vector multiplication

$(I_{m-1} + A^{(k+1)})^\top (I_{m-1} + A^{(k+1)})\mathbf{v}$  can be achieved efficiently by applying the fast algorithm, FFT, to the Toeplitz-like structure of the resulting matrix  $A^{(k+1)}$  with  $\mathcal{O}((m-1)\log(m-1))$  operations. Similarly, from Eq. (19), we know that the solution of  $(P_\ell^{(k+1)})^\top P_\ell^{(k+1)}\mathbf{w} = \mathbf{z}$  can be obtained with only  $\mathcal{O}((m-1)\ell)$  operations.

#### 4. Numerical experiments

In this section, we present an example to compare the performances of preconditioned iterative methods versus unconditioned iterative methods. For all methods, the initial values are chosen to be

$$\mathbf{v}_0 = \begin{cases} \mathbf{u}^{(0)} := [\phi(x_1), \dots, \phi(x_{m-1})]^\top, & k = 1, \\ 2\mathbf{u}^{(k)} - \mathbf{u}^{(k-1)}, & k > 1, \end{cases}$$

as suggested in [27], and the stopping criterion is

$$\frac{\|\mathbf{r}_j\|_2}{\|\mathbf{b}^{(k+1)}\|_2} < 10^{-7},$$

where  $\mathbf{r}_j$  is the residual vector after the  $j$ th iteration.

**Example 4.1.** Consider the problem in Eq. (1) with  $\alpha = 0.8$ ,  $\beta = 0.6$ , and  $\gamma = 1.8$ . The left-sided and right-sided diffusion coefficients are given by

$$\begin{aligned} d_+(x, t) &= 6(1+t)x^{0.6}, & d_-(x, t) &= 6(1+t)(1-x)^{0.6}, \\ e_+(x, t) &= 6(1+t)x^{1.8}, & e_-(x, t) &= 6(1+t)(1-x)^{1.8}, \end{aligned}$$

with the spatial interval  $\Omega = (0, 1) \times (0, 1)$  and the time interval  $[0, T] = [0, 1]$ . The source term and initial condition are given by

$$\begin{aligned} f(x, t) &= e^t \left[ 6(1+t) \left( \left( \frac{\Gamma(4)}{\Gamma(3.4)} - \frac{\Gamma(4)}{\Gamma(2.2)} \right) (x^3 + (1-x)^3) - \left( \frac{3\Gamma(5)}{\Gamma(4.4)} - \frac{3\Gamma(5)}{\Gamma(3.2)} \right) (x^4 + (1-x)^4) \right. \right. \\ &\quad \left. \left. + \left( \frac{3\Gamma(6)}{\Gamma(5.4)} - \frac{3\Gamma(6)}{\Gamma(4.2)} \right) (x^5 + (1-x)^5) - \left( \frac{\Gamma(7)}{\Gamma(6.4)} - \frac{\Gamma(7)}{\Gamma(5.2)} \right) (x^6 + (1-x)^6) \right) + x^3(1-x)^3 \right] \end{aligned}$$

and

$$u(x, 0) = x^3(1-x)^3.$$

By direct computation, we can show that the solution to the fractional diffusion equation is

$$u(x, t) = e^t x^3(1-x)^3.$$

We obtained the numerical results using MATLAB R2010a on a Lenovo Laptop Intel(R) Core(TM)2 Duo with a 2.20 GHz CPU and 2-GB RAM. We set the bandwidth  $\ell$  of the preconditioner  $P_\ell^{(k+1)}$  equal to 8 and use “ $m$ ” and “ $n$ ” to represent the numbers of the spatial partition and the number of the temporal partition, respectively. In Tables 1 and 2, we present the average numbers of iterations and the CPU times (seconds) required by the GMRES(20), PGMRES(20), CGNR, and PCGNR methods. We see that the number of iterations and the execution time by the GMRES(20) and CGNR methods increase dramatically, while those by the PGMRES(20) and PCGNR methods are changed very little. The

Table 1: The average number of iterations for Example 4.1

$m = n$	GMRES(20)	PGMRES(20)	CGNR	PCGNR
16	8.000	3.063	12.438	3,125
32	16.000	3.938	32.594	4.063
64	84.969	4.063	100.547	4.813
128	231.781	5.055	318.852	4.797
256	486.859	6.082	1060.191	5.148

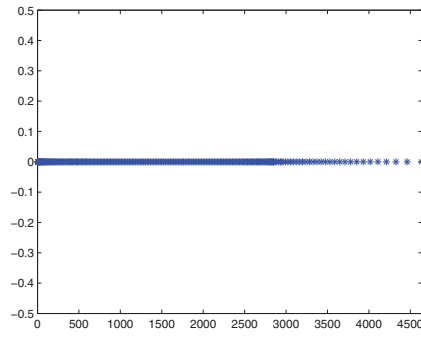
Table 2: The required CPU times for Example 4.1

$m = n$	GMRES(20)	PGMRES(20)	CGNR	PCGNR
16	0.0046	0.0310	0.0620	0.0320
32	0.1400	0.0470	0.2810	0.0780
64	1.4510	0.1560	1.7000	0.1870
128	10.9200	0.5930	18.2210	0.7330
256	55.5830	3.7120	162.7550	4.1340

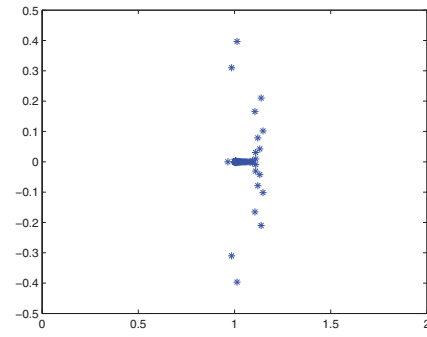
phenomena might be explained by the clustering of the eigenvalues of the relevant coefficient matrices. As an example, Figure 1 shows the distribution of the eigenvalues of matrices  $\hat{A}$ ,  $\hat{A}^\top \hat{A}$ ,  $(P_8^{(1)})^{-1} \hat{A}$  and  $((P_8^{(1)})^\top P_8^{(1)})^{-1} \hat{A}^\top \hat{A}$  with  $m = n = 256$ . Also, Table 3 indicates the effect of the preconditioners on the condition numbers of the relevant matrices. Note that the condition number significantly improves with the help of the proposed preconditioners. Figure 2 shows the behavior of the exact solution and the numerical solution with  $m = n = 256$ . As shown in the figure, once the computation is terminated, it recovers the shape of the original function. Specifically, using the sup-norm and the PGMRES methods, the errors computed between the true and numerical solutions at the last time step are  $4.6312 \times 10^{-4}$ ,  $2.4162 \times 10^{-4}$ ,  $7.5522 \times 10^{-5}$ , and  $4.5765 \times 10^{-5}$  for matrices of sizes 16, 31, 64, 128, and 256, respectively.

Table 3: Condition numbers for relevant matrices for Example 4.1.

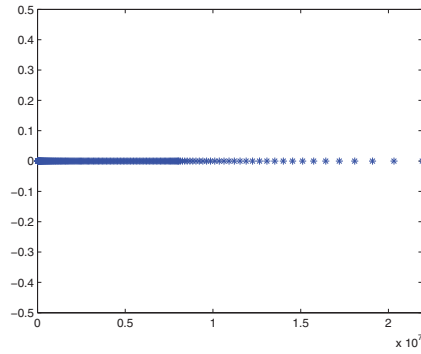
$m = n$	16	32	64	128	256
$k(\hat{A})$	48.86	162.84	491.07	1.34e+3	3.34e+3
$k((P_8^{(1)})^{-1}\hat{A})$	1.05	1.17	1.29	1.47	1.79
$k(\hat{A}^\top \hat{A})$	2.39e+3	2.65e+4	2.41e+5	1.79e+6	1.16e+7
$k(((P_8^{(1)})^\top P_8^{(1)})^{-1} \hat{A}^\top \hat{A})$	1.88	20.65	193.57	960.76	3.46e+3



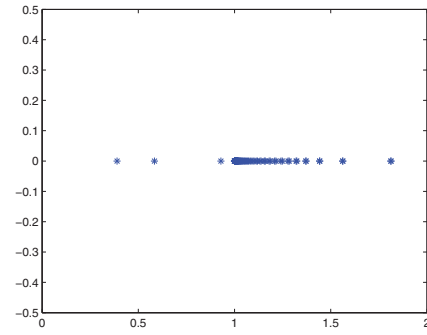
(a) Spectrum of  $\hat{A}$



(b) Spectrum of  $(P_8^{(1)})^{-1}\hat{A}$



(c) Spectrum of  $\hat{A}^\top \hat{A}$



(d) Spectrum of  $((P_8^{(1)})^\top P_8^{(1)})^{-1} \hat{A}^\top \hat{A}$

Figure 1: The spectra of the unpreconditioned and preconditioned coefficient matrices at time  $t_1$  with  $m = n = 256$ .



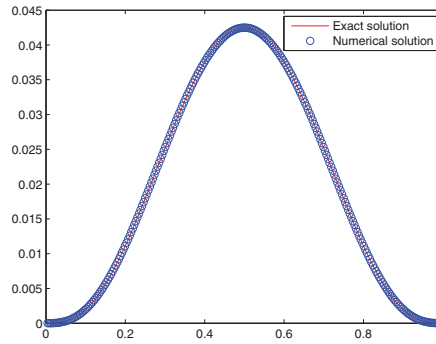


Figure 2: Numerical and exact solutions at time  $t_n$  with  $m = n = 256$ .

## 5. Conclusion

Determining analytic solutions for FDEs is very challenging and solutions remain unknown for most FDEs. This paper presents an implicit approach for solving STFDEs with two-sided Grünwald formulae. More significantly, with the aid of Eq. (15), we can improve the calculation skill by the implementation of efficient and reliable preconditioning iterative techniques, the PGMRES and PCGNR methods, incurring only the computational cost of  $\mathcal{O}((m-1)\log(m-1))$ . Our numerical results strongly suggest the efficiency of the proposed preconditioning methods.

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