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On single-step HSS iterative method with circulant preconditioner for fractional diffusion equations

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Abstract

By exploiting Toeplitz-like structure and non-Hermitian dense property of the discrete coefficient matrix, a new double-layer iterative method called SHSS-PCG method is employed to solve the linear systems originating from the implicit finite difference discretization of fractional diffusion equations (FDEs). The method is a combination of the single-step Hermitian and skew-Hermitian splitting (SHSS) method with the preconditioned conjugate gradient (PCG) method. Further, the new circulant preconditioners are proposed to improve the efficiency of SHSS-PCG method, and the computation cost is further reduced via using the fast Fourier transform (FFT). Theoretical analysis shows that the SHSS-PCG iterative method with circulant preconditioners is convergent. Numerical experiments are given to show that our SHSS-PCG method with circulant preconditioners preforms very well, and the proposed circulant preconditioners are very efficient in accelerating the convergence rate.

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1 Introduction

Fractional calculus has a long history and its origin goes back to describing half order ($\alpha = 1/2$) derivative by Leibnitz in 1695. It was believed that this branch of mathematics had no applications. But in the last thirty years, the fractional derivatives and the fractional partial differential equations (FPDEs) have attracted growing attention [1, 2], because they can provide an adequate and accurate description of transport processes that exhibit anomalous diffusion behavior in the real word [3, 4], including Brownian motion, entropy [5], groundwater contaminant transport [6, 7], turbulent flow [8, 9], and applications in biology [10], image processing [11], engineering and physics [12–15].

In recent years, a large amount of work has been devoted to finding out how to solve FPDEs [16–18]. The main reason is that it is more challenging or sometimes even impossible to obtain the analytical solution of FPDEs, or that the obtained analytical solution is less valuable (expressed by the transcendental functions or infinite series). As a consequence, numerical solutions for FPDEs have become the main methods and then have

been developed intensively, e.g., (compact) finite difference methods [19–22], finite element methods [23, 24], discontinuous Galerkin methods [25, 26], and other numerical methods [27–29].

However, due to the nonlocality of a fractional differential operator, a naive discretization of FDEs, even though implicit, leads to unconditional instability [30, 31]. Moreover, coefficient matrices arising from most numerical discretizations of FDEs are non-sparse and typically require the computational cost of $O(N^3)$ by using Gaussian elimination and the storage of $O(N^2)$, where N is the number of grid points [32].

In order to overcome the difficulty of stability, Meerschaet and Tadjeran [30, 31] proposed an unconditionally stable shifted Grünwald discretization to approximate the FDEs, which is based on the equivalence of Grünwald–Letnikov fractional derivative and Riemann–Liouville fractional derivative with some conditions. Later, the Toeplitz-like structure of the full coefficient matrix via Meerschaet–Tadjeran's method was discovered [32, 33]; more precisely, such a full matrix can be written as the sum of diagonal-multiply-Toeplitz matrices. Thus, the storage is significantly reduced from $O(N^2)$ to $O(N)$ and the matrix-vector multiplication of Toeplitz matrix can be calculated by using the fast Fourier transform (FFT) with $O(N \log N)$ operations [34–36]. By exploiting such a special structure, Wang and Wang [37] proposed the conjugate gradient normal residual (CGNR) method to solve the discretized system of FDEs with Meerschaet–Tadjeran's method, and numerically showed that its convergence is fast with smaller diffusion coefficients (in that case the discretized system is well-conditioned). On the other hand, when the diffusion coefficients are not small, the problem becomes ill-conditioned and the convergence of the CGNR method slows down. To avoid the resulting drawback, Lei and Sun [38] proposed a robust CGNR method with the circulant preconditioner to solve the FDEs with Meerschaet–Tadjeran's method under the condition that the diffusion coefficients are constant and the ratio $\frac{\Delta x^\alpha}{\Delta t}$ is bounded away from zero. The spectrum of the preconditioned matrix is proven to cluster around 1 if the diffusion coefficients are constant and the convergence rate of the proposed iterative algorithm is superlinear. In 2015, Bai, Huang, and Gu [39] proposed the Hermitian and skew-Hermitian splitting methods and the circulant preconditioner to accelerate the convergence rate for solving the fractional diffusion equations with constant coefficients; and numerical results show that the methods and circulant preconditioners are efficient.

The novelty of this paper is to present a new double-layer SHSS-PCG iterative method to further utilize matrix structure to improve the computational efficiency for solving the full non-Hermitian linear systems originating in the discretization of FDEs. The new method includes two aspects. One is that the outer iteration is a single-step HSS (SHSS) iterative method to utilize the fact that the coefficient matrix generated by Meerschaet–Tadjeran's method is a full non-Hermitian positive definite matrix and its Hermitian part is dominant; and the other is that the inner iteration is the classic conjugate gradient (CG) method with circulant preconditioners based on Strang's and T. Chan's approximation, to take the full advantage of the Toeplitz structure of the dominant Hermitian part.

The rest of the present paper is organized as follows: In Sect. 2, we briefly introduce the Meerschaet–Tadjeran discretization for the FDEs. In Sect. 3, the SHSS-PCG iterative method is proposed for solving the discretized Toeplitz-like linear systems. In Sect. 4, the convergence of the SHSS-PCG iterative method with circulant preconditioners is dis-

cussed. In Sect. 5, numerical experiments are given to show the performance of the proposed method. Finally, some concluding remarks are given in Sect. 6.

2 FDEs and finite difference discretization

In this paper, we consider the following initial-boundary value problem of FDEs:

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} = d_+(x,t)\frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} + d_-(x,t)\frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} + f(x,t), \\ (x,t) \in (x_L, x_R) \times (0,T], \\ u(x,0) = u_0(x), \quad x \in [x_L, x_R], \\ u(x_L,t) = u(x_R,t) = 0, \quad t \in [0,T], \end{cases} \tag{1}$$

where $\alpha \in (1,2)$ is the order of the fractional derivative, $f(x,t)$ is the source/sink term, and the diffusion coefficient functions $d_\pm(x,t)$ are nonnegative, i.e., $d_\pm(x,t) \geq 0$.

When $\alpha = 2$, and setting $d(x,t) = d_+(x,t) + d_-(x,t)$, FDEs (1) become the classical parabolic PDEs. And when $\alpha = 1$, and setting $d(x,t) = d_+(x,t) - d_-(x,t)$, FDEs (1) reduce to the classical hyperbolic PDEs. The case $1 < \alpha < 2$ represents a super-diffusive process, where particles diffuse faster than the classical parabolic PDEs predict [30].

From a numerical point of view, an interesting definition of the right-sided and the left-sided fractional derivatives is the Grünwald–Letnikov form given by

$$\begin{aligned} \frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} &= \lim_{\Delta x \to 0^+} \frac{1}{\Delta x^\alpha} \sum_{k=0}^{\lfloor (x-x_L)/\Delta x \rfloor} g_k^{(\alpha)} u(x - k\Delta x, t), \\ \frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha} &= \lim_{\Delta x \to 0^+} \frac{1}{\Delta x^\alpha} \sum_{k=0}^{\lfloor (x_R-x)/\Delta x \rfloor} g_k^{(\alpha)} u(x + k\Delta x, t), \end{aligned}$$

where $\lfloor \cdot \rfloor$ denotes the floor function, and $g_k^{(\alpha)}$ is the alternating fractional binomial coefficient given as

$$\begin{aligned} &g_0^{(\alpha)} = 1, \qquad g_k^{(\alpha)} = \frac{(-1)^k}{k!}\alpha(\alpha-1)\cdots(\alpha-k+1), \quad \text{or} \\ &g_k^{(\alpha)} = \left(1 - \frac{(\alpha+1)}{k}\right) g_{k-1}^{(\alpha)}, \quad k = 1,2,3,\ldots. \end{aligned} \tag{2}$$

Let N and M be positive integers, and $\Delta x = \frac{x_R - x_L}{N+1}$ and $\Delta t = T/m$ be the sizes of spatial grid and time step, respectively. The spatial partition is defined as $x_i = x_L + i\Delta x$ for $i = 0,1,2,\ldots,N$ and the temporal partition is defined as $t_m = m\Delta t$ for $m = 0,1,2,\ldots,M$. The Meerschaet–Tadjeran's method is to combine a discretization in time of equation (1) with an implicit Euler method, and a discretization in space of the fractional derivatives with a shifted Grünwald estimate, i.e.,

$$\begin{aligned} \frac{u(x_i,t_m) - u(x_i,t_{m-1})}{\Delta t} &= d_+(x_i,t_m)\frac{\partial^\alpha u(x_i,t_m)}{\partial_+ x^\alpha} + d_-(x_i,t_m)\frac{\partial^\alpha u(x_i,t_m)}{\partial_- x^\alpha} \\ &\quad + f(x_i,t_m) + \mathcal{O}(\Delta t), \end{aligned}$$

where

$$\frac{\partial^\alpha u(x_i,t_m)}{\partial_+ x^\alpha} = \frac{1}{\Delta x^\alpha}\sum_{k=0}^{i+1} g_k^{(\alpha)} u(x_{i-k+1},t_m) + \mathcal{O}(\Delta x),$$

$$\frac{\partial^\alpha u(x_i,t_m)}{\partial_- x^\alpha} = \frac{1}{\Delta x^\alpha}\sum_{k=0}^{N-i+2} g_k^{(\alpha)} u(x_{i+k-1},t_m) + \mathcal{O}(\Delta x)$$

with $g_k^{(\alpha)}$ defined in (2); see [30, 31].

Let $u_i^{(m)} = u(x_i,t_m)$, $d_{\pm,i}^{(m)} = d_\pm(x_i,t_m)$ and $f_i^{(m)} = f(x_i,t_m)$, then the corresponding implicit finite difference scheme

$$\frac{u_i^{(m)} - u_i^{(m-1)}}{\Delta t} = \frac{d_{+,i}^{(m)}}{\Delta x^\alpha}\sum_{k=0}^{i+1} g_k^{(\alpha)} u_{i-k+1}^{(m)} + \frac{d_{-,i}^{(m)}}{\Delta x^\alpha}\sum_{k=0}^{N-i+2} g_k^{(\alpha)} u_{i+k-1}^{(m)} + f_i^{(m)}$$

is unconditionally stable. Let

$$u^{(m)} = \left[u_1^{(m)}, u_2^{(m)}, \ldots, u_N^{(m)}\right]^T, \qquad f^{(m)} = \left[f_1^{(m)}, f_2^{(m)}, \ldots, f_N^{(m)}\right]^T$$

and $I \in \mathbb{R}^{N\times N}$ be the identity matrix, then the numerical discrete scheme can be rewritten in a matrix form as follows (see [32]):

$$\left(\frac{\Delta x^\alpha}{\Delta t} I + A^{(m)}\right) u^{(m)} = \frac{\Delta x^\alpha}{\Delta t} u^{(m-1)} + \Delta x^\alpha f^{(m)} \tag{3}$$

with

$$A^{(m)} = D_+^{(m)} G_\alpha + D_-^{(m)} G_\alpha^T,$$

where $D_\pm^{(m)} = \operatorname{diag}(d_{\pm,1}^{(m)}, d_{\pm,2}^{(m)}, \ldots, d_{\pm,N}^{(m)})$ and

$$G_\alpha = -\begin{bmatrix} g_1^{(\alpha)} & g_0^{(\alpha)} & 0 & \cdots & 0 & 0 \\ g_2^{(\alpha)} & g_1^{(\alpha)} & g_0^{(\alpha)} & \ddots & \ddots & 0 \\ g_3^{(\alpha)} & g_2^{(\alpha)} & g_1^{(\alpha)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ g_{N-1}^{(\alpha)} & \ddots & \ddots & \ddots & g_1^{(\alpha)} & g_0^{(\alpha)} \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & \cdots & \cdots & g_2^{(\alpha)} & g_1^{(\alpha)} \end{bmatrix}_{N\times N}. \tag{4}$$

We must note that G_α is a Toeplitz matrix and that the coefficient matrix $A^{(m)}$ is a full Toeplitz-like matrix, which is asymmetric in general. Furthermore, the storage of Toeplitz-like $A^{(m)}$ can be reduced $O(N)$ and the matrix-vector multiplication can be obtained in $O(N\log N)$ operations via the FFT.

Denote

$$\nu_{N,M} = \frac{\Delta x^\alpha}{\Delta t} = \frac{(x_R - x_L)^\alpha}{(N+1)^\alpha}\frac{M}{T}, \tag{5}$$

which is related to the number of time steps and grid points. The linear system (3) can be written as

$$\mathcal{M}^{(m)}u^{(m)} = b^{(m-1)}, \quad b^{(m-1)} = \nu_{N,M}\big(u^{(m-1)} + \Delta t f^{(m)}\big), \tag{6}$$

where

$$\mathcal{M} = \nu_{N,M}I + A^{(m)} = \nu_{N,M}I + D_{+}^{(m)}G_{\alpha} + D_{-}^{(m)}G_{\alpha}^{T}.$$

3 SHSS-PCG iterative methods

In this section, we first introduce the single-step HSS (SHSS) iterative method, and then propose the SHSS-PCG iterative method for solving the discretized linear system (6).

Suppose that the diffusion coefficients are two nonnegative constants, i.e., $d_{+,i}^{(m)} = d_{+} \geq 0$, $d_{-,i}^{(m)} = d_{-} \geq 0$ and $d_{+} + d_{-} \neq 0$. Let $\mathcal{M}^{(m)} = H + S$, where

$$\begin{aligned} H &= \frac{1}{2}\big(\mathcal{M}^{(m)} + \mathcal{M}^{(m)^T}\big) = \nu_{N,M}I + \frac{d_{+} + d_{-}}{2}\big(G_{\alpha} + G_{\alpha}^{T}\big) \\ &= \nu_{N,M}I + \frac{d_{+} + d_{-}}{2}J_{H,N}, \end{aligned} \tag{7}$$

and

$$S = \frac{1}{2}\big(\mathcal{M}^{(m)} - \mathcal{M}^{(m)^T}\big) = \frac{d_{+} - d_{-}}{2}\big(G_{\alpha} - G_{\alpha}^{T}\big) = \frac{d_{+} - d_{-}}{2}J_{S,N}, \tag{8}$$

with

$$J_{H,N} = \begin{bmatrix} 2g_1^{(\alpha)} & g_0^{(\alpha)} + g_2^{(\alpha)} & g_3^{(\alpha)} & \cdots & g_{N-1}^{(\alpha)} & g_N^{(\alpha)} \\ g_2^{(\alpha)} + g_0^{(\alpha)} & 2g_1^{(\alpha)} & g_0^{(\alpha)} + g_2^{(\alpha)} & \cdots & g_{N-2}^{(\alpha)} & g_{N-1}^{(\alpha)} \\ g_3^{(\alpha)} & g_2^{(\alpha)} + g_0^{(\alpha)} & 2g_1^{(\alpha)} & \cdots & \cdots & g_{N-2}^{(\alpha)} \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ g_{N-1}^{(\alpha)} & g_{N-2}^{(\alpha)} & \cdots & \cdots & 2g_1^{(\alpha)} & g_0^{(\alpha)} + g_2^{(\alpha)} \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & g_{N-2}^{(\alpha)} & \cdots & g_2^{(\alpha)} + g_0^{(\alpha)} & 2g_1^{(\alpha)} \end{bmatrix},$$

$$J_{S,N} = \begin{bmatrix} 0 & g_0^{(\alpha)} - g_2^{(\alpha)} & -g_3^{(\alpha)} & \cdots & -g_{N-1}^{(\alpha)} & -g_N^{(\alpha)} \\ g_2^{(\alpha)} - g_0^{(\alpha)} & 0 & g_0^{(\alpha)} - g_2^{(\alpha)} & \cdots & -g_{N-2}^{(\alpha)} & -g_{N-1}^{(\alpha)} \\ g_3^{(\alpha)} & g_2^{(\alpha)} - g_0^{(\alpha)} & 0 & \cdots & \cdots & -g_{N-2}^{(\alpha)} \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ g_{N-1}^{(\alpha)} & g_{N-2}^{(\alpha)} & \cdots & \cdots & 0 & g_0^{(\alpha)} - g_2^{(\alpha)} \\ g_N^{(\alpha)} & g_{N-1}^{(\alpha)} & g_{N-2}^{(\alpha)} & \cdots & g_2^{(\alpha)} - g_0^{(\alpha)} & 0 \end{bmatrix}.$$

Obviously, the above matrix splitting is the Hermitian and skew-Hermitian splitting (HSS).

Based on this splitting, Li [40] proposed using the SHSS iterative method to solve linear system (6).

The SHSS method Given an initial guess $x^{(0)}$, for $k = 0, 1, 2, \ldots$, until $\{x^{(k)}\}$ converges, compute

$$(\beta I + H)x^{(k+1)} = (\beta I - S)x^{(k)} + b, \tag{9}$$

where β is a given positive constant, H and S are the Hermitian and skew-Hermitian parts of $\mathcal{M}^{(m)}$, respectively.

Obviously, the SHSS iterative method is a single step iterative scheme. The convergence of the SHSS is discussed in [40] and described in the following lemma.

Lemma 3.1 ([40]) *Let $\mathcal{M}^{(m)} \in \mathbb{C}^{n\times n}$ be a positive definite matrix, $H = \frac{1}{2}(\mathcal{M}^{(m)} + \mathcal{M}^{(m)^T})$ and $S = \frac{1}{2}(\mathcal{M}^{(m)} - \mathcal{M}^{(m)^T})$ be its Hermitian and skew-Hermitian parts, respectively. Let β be a positive constant. Then the spectral radius $\rho(T(\beta))$ of the iteration matrix $T(\beta) = (\beta I + H)^{-1}(\beta I - S)$ of the SHSS iterative method is bounded by $\delta_\beta = \frac{\beta^2+\sigma_{\max}^2}{\beta+\lambda_{\min}}$, where $\lambda_{\min}$ is the smallest eigenvalue of matrix H and $\sigma_{\max}^2$ is the largest singular value of matrix S. Moreover, it holds $\rho(T(\beta)) \le \delta_\beta \le 1$ when $\beta > \frac{\sigma_{\max}^2-\lambda_{\min}}{2\lambda_{\min}}$, i.e., the SHSS iterative method converges to the unique solution x^* of (6).*

Since it is very costly and impractical to obtain the exact solution, the linear problems in (9) are solved iteratively and approximately in practice. Considering $\beta I + H$ is Hermitian positive definite and its Toeplitz-like structure is exploited, we may employ the CG method with some circulant preconditioners to solve approximately the linear systems. Thus, we may obtain a new iterative method, called SHSS-PCG method.

More clearly, we rewrite this SHSS-PCG iterative method with circulant preconditioner P for solving the non-Hermitian full linear system (6) as the following scheme (Algorithm 1 and Subroutine 1).

Next, we introduce two circulant preconditioners for Toeplitz matrix $T = (t_{i-j})_{0\le i,j\le N}$. One is based on Strang's circulant approximation, called Strang's preconditioner $s(T)$ [41], which is defined to be the circulant matrix obtained by copying the central diagonal of T and then bringing them around to satisfy the circulant requirement. More precisely, the

Algorithm 1 SHSS-PCG for $\mathcal{M}^{(m)}u^{(m)} = b^{(m-1)}$ with circulant preconditioner P

1. Given an initial guess $u_0^{(m)} = 0$ and set $k = 0$;
2. Compute $r_0 = b^{(m-1)} - \mathcal{M}^{(m)}u_0^{(m)}$;
3. For $k = 0, 1, 2, \ldots$, until converges, do
   Solve $(\beta I + H)v_k = r_0$ by calling subroutine PCG ($(\beta I + H)$, r_0, Tol, Maxit, P);
   Set $u_{k+1}^{(m)} = u_k^{(m)} + v_k$, compute $r_{k+1} = b^{(m-1)} - \mathcal{M}^{(m)}u_{k+1}^{(m)}$;
4. End do.

Subroutine 1 PCG for $(\beta I + H)v_k = r_0$ with circulant preconditioner P

1. Given an initial guess $v_k = 0$, set $j = 0$;
2. Compute $z_0 = r_0 - (\beta I + H)v_k$ by using the FFT and set $p = z_0$;
3. For $j = 0, 1, 2, \ldots$, until converges, do
   Compute $w = (\beta I + H)p$, $w = P^{-1}w$ by using the FFT;
   Compute $\alpha = \frac{z_j^T z_j}{p^T w}$ and set $v_k = v_k + \alpha p$;
   Set $z_{j+1} = z_j - \alpha w$;
   Compute $\beta = \frac{z_{j+1}^T z_{j+1}}{z_j^T z_j}$ and set $p = z_{j+1} + \beta p$;
4. End do.

diagonal elements s_k of $s(T)$ are given by

$$s_k = \begin{cases} t_k, & 0 \le k < N/2, \\ 0, & k = N/2 \text{ is even}, \\ t_{k-N}, & N/2 < k \le N-1, \\ s_{k+N}, & 0 \le -k \le N-1. \end{cases}$$

The other is based on T. Chan's circulant approximation, called T. Chan's preconditioner $c(T)$ [42], whose diagonal elements are given by

$$c_k = \begin{cases} \frac{(N-k)t_k + kt_{k-N}}{N}, & 0 \le k \le N-1, \\ c_{N+k}, & 0 < -k \le N-1. \end{cases}$$

Recall that $\beta I + H = (\beta + \nu_{N,M})I + \frac{d_+ + d_-}{2} J_{H,N}$, and $J_{H,N} = (G_\alpha + G_\alpha^T)$ is the Toeplitz matrix given in (7), then Strang's circulant preconditioner is defined as

$$s(\beta I + H) = (\beta + \nu_{N,M})I + \frac{d_+ + d_-}{2} s(J_H), \tag{10}$$

where Strang's circulant matrix $s(J_H)$ is determined by only n entries lying in the first column and is further denoted as

$$s(J_{H,N}) = \operatorname{circ}\bigl(2g_1^{(\alpha)}, g_2^{(\alpha)} + g_0^{(\alpha)}, g_3^{(\alpha)}, \ldots, g_{\lfloor \frac{N+1}{2} \rfloor}^{(\alpha)}, 0, g_{\lfloor \frac{N+1}{2} \rfloor}^{(\alpha)}, \ldots, g_3^{(\alpha)}, g_2^{(\alpha)} + g_0^{(\alpha)}\bigr).$$

And T. Chan's circulant preconditioner is defined as

$$c(\beta I + H) = (\beta + \nu_{N,M})I + \frac{d_+ + d_-}{2} c(J_H), \tag{11}$$

where $c(J_H)$ is T. Chan's circulant matrix of J_H, and determined by only n entries lying in the first column, which is further denoted as

$$\begin{aligned} c(J_{H,N}) = \frac{1}{N} \operatorname{circ}\bigl(&2Ng_1^{(\alpha)}, (N-1)\bigl(g_2^{(\alpha)} + g_0^{(\alpha)}\bigr) + g_N^{(\alpha)}, (N-2)\bigl(g_3^{(\alpha)}\bigr) + 2g_N^{(\alpha)}, \\ &\cdots\cdots, g_N^{(\alpha)} + (N-1)\bigl(g_2^{(\alpha)} + g_0^{(\alpha)}\bigr)\bigr). \end{aligned}$$

A circulant matrix C can be diagonalized by the discrete Fourier matrix F, i.e., $F^* C F = \Lambda$, where the entries of Fourier matrix F are given by

$$F_{j,k} = \frac{1}{\sqrt{N}} \exp\left(\frac{2\pi \mathrm{i}}{N} jk\right), \quad 0 \le j, k, \le N-1$$

with the imaginary unit i, and Λ is a diagonal matrix formed by the eigenvalues of C, which can be obtained in $O(N \log N)$ operations by using the FFT [35]. Further, since $C = F^* \Lambda F$, then $C^T = F^* \overline{\Lambda} F$, where $\overline{\Lambda}$ is the complex conjugate of Λ. That is to say, the eigenvalues of circulant matrix C^T are just equal to the complex conjugation of the eigenvalues of circulant matrix C.

4 Spectrum of the preconditioned matrix

In this section, we study the convergence rate of the SHSS-PCG method with the proposed circulant preconditioners $s(\beta I + H)$ and $c(\beta I + H)$ for solving the linear system (6). Firstly, some useful properties of the alternating fractional binomial coefficient $g_k^{(\alpha)}$ are summarized in the following; see [30–32].

Lemma 4.1 *Let $1 < \alpha < 2$, the following properties of the coefficients $g_k^{(\alpha)}$ defined in (2) are satisfied*:

$$g_0^{(\alpha)} = 1, \qquad g_1^{(\alpha)} = -\alpha < 0, \qquad 1 > g_2^{(\alpha)} > g_3^{(\alpha)} > \cdots > 0,$$

$$\sum_{k=0}^{\infty} g_k^{(\alpha)} = 0, \qquad \sum_{k=0}^{n} g_k^{(\alpha)} < 0, \quad \forall n \geq 1.$$

Lemma 4.2 *All eigenvalues of $s(J_{H,N})$ and $c(J_{H,N})$ fall inside the open disc $\{z \in \mathbb{C} : |z - 2\alpha| < 2\alpha\}$.*

Proof According the properties of the sequence $\{g_k^{(\alpha)}\}$ and $J_{H,N} = G_\alpha + G_\alpha^T$, all the Gershgorin disc of the circulant matrices $s(J_{H,N})$ is centered at $-2g_1^{(\alpha)} = 2\alpha$ with radius

$$r_N^s = 2\left(g_0^{(\alpha)} + g_2^{(\alpha)} + \sum_{k=3}^{\lfloor \frac{N+1}{2} \rfloor} g_k^{(\alpha)}\right) < 2\sum_{k=0,k\neq 1}^{\infty} g_k^{(\alpha)} = -2g_1^{(\alpha)} = 2\alpha,$$

and all the Gershgorin disc of the circulant matrices $c(J_{H,N})$ is centered at $-2g_1^{(\alpha)} = 2\alpha$ with radius

$$\begin{aligned} r_N^c &= 2\left(\frac{(N-1)(g_0^{(\alpha)} + g_2^{(\alpha)}) + g_N^{\alpha}}{N} + \sum_{k=3}^{N-1} \frac{(N-k+1)g_k^{(\alpha)} + (k-1)g_{N-k}^{(\alpha)}}{N}\right) \\ &< 2\frac{N-1}{N}\sum_{k=0,k\neq 1}^{N} g_k^{(\alpha)} < 2\frac{N-1}{N}\sum_{k=0,k\neq 1}^{\infty} g_k^{(\alpha)} < -2g_1^{(\alpha)} = 2\alpha. \end{aligned}$$

□

Proposition 4.3 *The eigenvalues of $s(J_{H,N})$ and $c(J_{H,N})$ are all positive real numbers and bound above by $4\alpha < 8$ for all N.*

Secondly, the invertibility of preconditioners $s(\beta I + H)$ and $c(\beta I + H)$ are discussed.

Theorem 4.4 *Let $1 < \alpha < 2$. The preconditioners $s(\beta I + H)$ in (10) and $c(\beta I + H)$ in (11) are invertible and the norm of their inverses is bound by $\frac{1}{\beta + \nu_{N,M}}$.*

Proof Since H in (7) is Hermitian, by Proposition 4.3, the eigenvalues of $s(J_{H,N})$ and $c(J_{H,N})$ are all positive real numbers and bound above 8. Noting that $\nu_{N,M} > 0$ and $d_\pm > 0$, we have

$$[\Lambda_{s(\beta I+H)}]_{k,k} = \beta + \nu_{N,M} + \frac{d_- + d_+}{2}[\Lambda_{s(J_{H,N})}]_{k,k} \geq \beta + \nu_{N,M} > 0$$

and

$$[\Lambda_{c(\beta I+H)}]_{k,k} = \beta + \nu_{N,M} + \frac{d_- + d_+}{2}[\Lambda_{c(J_{H,N})}]_{k,k} \geq \beta + \nu_{N,M} > 0$$

for each $k = 1, 2, \ldots, N$. Therefore, $s(\beta I + H)$ in (10) and $c(\beta I + H)$ in (11) are invertible, and

$$\begin{aligned}
\left\| s(\beta I + H) \right\| &= \frac{1}{\min_{1 \le k \le N} |[\Lambda_{s(\beta I + H)}]|} < \frac{1}{\beta + \nu_{N,M}}, \\
\left\| c(\beta I + H) \right\| &= \frac{1}{\min_{1 \le k \le N} |[\Lambda_{c(\beta I + H)}]|} < \frac{1}{\beta + \nu_{N,M}}.
\end{aligned}$$

□

Theorem 4.5 *Let* $1 < \alpha < 2$ *and* $\bar{d} = \max(d_+, d_-)$. *The norm of the preconditioners* $s(\beta I + H)$ *in* (10) *and* $c(\beta I + H)$ *in* (11) *are bound by* $\beta + \nu_{N,M} + 8\bar{d}$.

Proof For any $k = 1, 2, \ldots, N$, by Proposition 4.3 and the fact that H is Hermitian, we have

$$\begin{aligned}
[\Lambda_{s(\beta I + H)}]_{k,k} &= \beta + \nu_{N,M} + \frac{d_- + d_+}{2} [\Lambda_{s(J_{H,N})}]_{k,k} \\
&< \beta + \nu_{N,M} + 8\frac{d_- + d_+}{2} < \beta + \nu_{N,M} + 8\bar{d}, \\
[\Lambda_{c(\beta I + H)}]_{k,k} &= \beta + \nu_{N,M} + \frac{d_- + d_+}{2} [\Lambda_{c(J_{H,N})}]_{k,k} \\
&< \beta + \nu_{N,M} + 8\frac{d_- + d_+}{2} < \beta + \nu_{N,M} + 8\bar{d}
\end{aligned}$$

for each $k = 1, 2, \ldots, N$. Therefore, the norm of $s(\beta I + H)$ in (10) $c(\beta I + H)$ in (11) is bound by $\beta + \nu_{N,M} + 8\bar{d}$.

Lastly, we consider the spectrum of preconditioned matrix $P^{-1}(\beta I + H)$, where P is the preconditioner $s(\beta I + H)$ or $c(\beta I + H)$.

We first introduce the generating function of the sequence of Toeplitz matrix $\{T_n\}_{n=1}^{\infty}$ [34]:

$$p(\theta) = \sum_{k=-\infty}^{\infty} t_k e^{\mathrm{i}k\theta},$$

where t_k is the kth diagonal of T_n. The generating function $p(\theta)$ is in the Wiener class if and only if $\sum_{-\infty}^{\infty} |t_k| < \infty$.

For $J_{H,N}$ defined in (7), we have

$$p(\theta) = \sum_{k=-\infty}^{\infty} t_k e^{\mathrm{i}k\theta} = -2 \sum_{k=-1}^{\infty} g_{k+1}^{(\alpha)} e^{\mathrm{i}k\theta}.$$

However, we must note that $\beta + \nu_{N,M} + \frac{d_- + d_+}{2} p(\theta)$ cannot be a generating function of $(\beta I + H)$ since $\nu_{N,M}$ is not independent on N. □

Lemma 4.6 ([38]) *Let* $p(\theta)$ *be the generating function of* $\{s(J_{H,N})\}_{N=1}^{\infty}$, *we have* $p(\theta)$ *is real-valued and nonnegative and in the Wiener class.*

Lemma 4.7 ([38]) *If the generating functions* $p(\theta)$ *of* $\{J_{H,N}\}_{N=1}^{\infty}$ *are in the Wiener class, then for any* ϵ, *there exist* $N', M' > 0$ *such that, for all* $N > N'$, $J_{H,N} - s(J_{H,N}) = U_N + V_N'$, *where* $\operatorname{rank}(U_N) \le M'$ *and* $\|V_N\| < \epsilon$.

Now we consider the spectrum of $(s(\beta I + H))^{-1}(\beta I + H) - I$.

Theorem 4.8 *Suppose the generating functions $p(\theta)$ of $\{J_{H,N}\}_{N=1}^{\infty}$ are in the Wiener class. For any ϵ, there exist $N'', M'' > 0$ such that, for all $N > N''$, $(s(\beta I + H))^{-1}(\beta I + H) - I = \widetilde{U}_N + \widetilde{V}_N$, where $\operatorname{rank}(U_N) \le M''$ and $\|V_N\|_2 < \epsilon$. That is to say, at most M'' eigenvalues of $(s(\beta I + H))^{-1}(\beta I + H) - I$ have absolute values larger than ϵ.*

Proof By Lemma 4.7, we have

$$\begin{aligned}
&\big(s(\beta I + H)\big)^{-1}(\beta I + H) - I \\
&\quad = \big(\beta I + s(H)\big)^{-1}\left(\beta I + \nu_{N,M} + \frac{d_+ + d_-}{2}J_{H,N} - \beta I - \nu_{N,M} - \frac{d_+ + d_-}{2}s(J_{H,N})\right) \\
&\quad = \frac{d_+ + d_-}{2}\big(\beta I + s(H)\big)^{-1}\big(J_{H,N} - s(J_{H,N})\big) \\
&\quad = \frac{d_+ + d_-}{2}\big(\beta I + s(H)\big)^{-1}\big(U_N + V_N'\big).
\end{aligned}$$

Note that $\operatorname{rank}((\beta I + s(H))^{-1}U_N) \le \operatorname{rank}(U_N) \le M'$ and $\|(\beta I + s(H))^{-1}V_N'\| \le \|(\beta I + s(H))^{-1}\|\,\|V_N'\| \le \frac{\epsilon}{\beta+\nu_{N,M}}$.

Thus, we complete the proof. □

Lemma 4.9 ([36]) *Let $J_{H,N}$ be given in (7) with a generating function $p(\theta)$ in the Wiener class. Then $\lim_{n\to\infty}\rho[s(J_{H,N}) - c(J_{H,N})] = 0$, where $\rho[\cdot]$ denotes the spectral radius.*

By using Theorem 4.8 and Lemma 4.9, we have the following theorem.

Theorem 4.10 *Let $J_{H,N}$ be given in (7) with a generating function $p(\theta)$ in the Wiener class. Then, for any ϵ, there exist $N'', M'' > 0$ such that, for all $N > N''$, $(c(\beta I + H))^{-1}(\beta I + H) - I = \widetilde{U}_N + \widetilde{V}_N$, where $\operatorname{rank}(U_N) \le M''$ and $\|V_N\|_2 < \epsilon$. That is to say, at most M'' eigenvalues of $(c(\beta I + H))^{-1}(\beta I + H) - I$ have the absolute values larger than ϵ.*

As a consequence, the spectrum of $(s(\beta I + H))^{-1}(\beta I + H)$ and $(c(\beta I + H))^{-1}(\beta I + H)$ clusters around 1 except for at most M'' outlying eigenvalues which are also bound. By Theorems 4.8 and 4.10, we know that the number of iterations is independent of N, and the convergence rate will be fast and superlinear when the PCG method is applied to solving $\mathcal{M}^{(m)}u^{(m)} = b^{(m-1)}$. We further recall that the algorithm requires $O(N \log N)$ operations in each iteration.

5 Numerical experiments

In this section, we solve FDEs (1) numerically by the implicit finite difference method given in Sect. 2. After the finite difference discretization, at each time step, the nonsymmetric linear system $\mathcal{M}^{(m)}u^{(m)} = b^{(m-1)}$ is solved by the proposed SHSS-PCG method with nonpreconditioner, Strang's and T. Chan's circulant preconditioners, respectively. The number of iterations required for convergence, CPU time, and the approximation under the infinity norm are reported to show the performances of the SHSS-PCG method. All numerical experiments are performed in MATLAB 8.1 (R2013a) in double precision on a

personal computer with 3.20 GHz CPU (Intel(R) Core(TM) i5-3470), 8.00 GB RAM, and Windows 7 operating system.

In our experiments, all tests are started from the zeros vector and terminated once the stopping criterion $\frac{\|r_k\|_2}{\|r_0\|_2} < 10^{-7}$ is satisfied, while the inner PCG iterations in the outer SHSS iteration are terminated if the current residuals of the inner iterations satisfy $\frac{\|p_j\|_2}{\|r_k\|_2} < 10^{-3}$, where p_j is the residual vector of the jth inner PCG iterations at the $(k+1)$th outer SHSS iteration, r_k is the residual vector of the kth outer SHSS iterate, and the initial guess at each time step is also chosen as the zero vector. Moreover, to improve the computational efficiency, all matrix vector multiplications Av are done by using the FFT in $O(N \log N)$ operations.

To this end, we consider the initial-boundary value problem of FDE (1) with source term $f(x,t) = 0$ for order of fractional derivatives $\alpha = 1.2$, 1.5, and 1.8. The spatial domain is $[x_L, x_R] = [0,2]$, and the time interval is $[0,T] = [0,1]$. The initial condition $u(x,0)$ is the following Gaussian pulse function:

$$u(x,0) = \exp\left(-\frac{(x-x_c)^2}{2\sigma^2}\right), \quad x_c = 1.5, \sigma = 0.08,$$

and the diffusion coefficients $d_+(x,t) \equiv 0.6$ and $d_-(x,t) \equiv 0.5$. That is,

$$\begin{cases} \frac{\partial u(x,t)}{\partial t} = 0.6 \times \frac{\partial^\alpha u(x,t)}{\partial_+ x^\alpha} + 0.5 \times \frac{\partial^\alpha u(x,t)}{\partial_- x^\alpha}, & (x,t) \in (x_L, x_R) \times (0,T], \\ u(x,0) = \exp(-\frac{(x-x_c)^2}{2\sigma^2}), & x_c = 1.5, \sigma = 0.08, \\ u(x_L,t) = u(x_R,t) = 0, & t \in [0,2]. \end{cases}$$

In the implementations, we adopt the experimentally optimal parameter $\beta = 0.01$ for the SHSS-PCG iteration. Numerical results are given in Tables 1–3. In these tables, we use "Non" for non-preconditioned method, "T. Chan" for T. Chan's circulant preconditioner, and "Strang" for Strang's circulant preconditioner. "N" denotes the number of spatial grid points, "$M = \lfloor ((N+1)^\alpha T \nu_{N,M})/(x_R - x_L)^\alpha \rfloor$" denotes the number of time steps and taking $\nu_{N,M} = 1$, "ERR" denotes the error between the true solution and the approximation under the infinity norm, "CPU (s)" denotes the total CPU time in seconds, and "IT" denotes the average number of iterations required for solving the FDE, i.e., IT $= \frac{1}{M}\sum_{m=1}^{M} \text{iter}(m)$, where iter$(m)$ denotes the number of iterations required for solving the linear systems.

Table 1 Numerical results of the SHSS-PCG method for solving FDE ($\alpha = 1.2$)

$N+1$	M	Pre.	IT_{SHSS}	IT_{PCG}	CPU (s)	ERR
2^8	339	Non	7.5	10.3	1.1352	2.1E–08
		T. Chan	7.5	7.1	0.8362	2.1E–08
		Strang	7.5	7.1	0.8148	2.1E–08
2^9	777	Non	7.2	10.2	3.3909	1.7E–08
		T. Chan	7.2	7.1	2.5087	1.7E–08
		Strang	7.2	7.1	2.5267	1.7E–08
2^{10}	1784	Non	6.6	10.1	11.6483	7.0E–08
		T. Chan	6.6	7.0	8.6258	7.2E–08
		Strang	6.6	7.0	8.8675	7.3E–08
2^{11}	4098	Non	6.5	9.8	48.6901	1.2E–07
		T. Chan	6.5	6.8	36.0236	1.5E–07
		Strang	6.5	6.8	35.4271	1.5E–07

Table 2 Numerical results of the SHSS-PCG method for solving FDE ($\alpha = 1.5$)

$N+1$	M	Pre.	$\mathrm{IT}_{\mathrm{SHSS}}$	$\mathrm{IT}_{\mathrm{PCG}}$	CPU (s)	ERR
2^8	1456	Non	5.1	10.8	3.4127	1.8E–08
		T. Chan	5.1	7.2	2.4424	1.8E–08
		Strang	5.1	7.3	2.4540	1.8E–08
2^9	4108	Non	4.9	10.3	13.2000	6.3E–08
		T. Chan	4.9	6.9	10.5790	6.2E–08
		Strang	4.9	6.9	9.1063	6.2E–08
2^{10}	11,602	Non	4.9	9.9	54.7901	2.7E–07
		T. Chan	4.9	6.4	38.3217	2.6E–07
		Strang	4.9	6.4	39.2306	2.6E–07
2^{11}	32,792	Non	4.1	9.0	222.3530	8.5E–06
		T. Chan	4.1	5.4	158.7036	7.8E–06
		Strang	4.1	5.4	151.6013	7.8E–06

Table 3 Numerical results of the SHSS-PCG method for solving FDE ($\alpha = 1.8$)

$N+1$	M	Pre.	$\mathrm{IT}_{\mathrm{SHSS}}$	$\mathrm{IT}_{\mathrm{PCG}}$	CPU (s)	ERR
2^8	6252	Non	4.0	9.5	10.4430	8.7E–07
		T. Chan	4.0	5.3	6.3253	8.7E–07
		Strang	4.0	5.1	6.0853	8.7E–07
2^9	21,694	Non	4.0	8.6	44.4843	3.1E–06
		T. Chan	4.0	4.6	26.9088	3.1E–06
		Strang	4.0	4.6	26.8528	3.1E–05
2^{10}	75,413	Non	4.0	7.6	230.6453	1.1E–05
		T. Chan	4.0	4.0	140.1736	1.1E–05
		Strang	4.0	4.0	141.2357	1.1E–05
2^{11}	262,374	Non	4.0	6.4	1324.4353	3.7E–05
		T. Chan	4.0	3.8	888.2863	3.7E–05
		Strang	4.0	3.8	899.8794	3.7E–05

From these tables, one can see that all experimented methods can successfully produce approximate solution to the full non-symmetric linear systems. When N increases, the number of iteration steps is either fixed or decreases slightly, but the amount of total CPU times increases. When the order of fractional derivative α becomes large, the number of iteration steps decreases slightly, but the amount of CPU time increases significantly.

Further, with two classic circulant preconditioners, the number of iterations and the amount of CPU time decrease rapidly, and are half of those of the SHSS-PCG method with non-preconditioner.

We must note that the efficiency of preconditioners employed in the proposed SHSS-PCG method is lower. The reason is that the number of inner iterations in the SHSS-PCG is small, which means that there is not enough space to improve the efficiency of preconditioner for the SHSS-PCG method.

6 Concluding remarks

In this paper, we focus our attention on the full Toeplitz-like structure and non-Hermitian property of coefficient matrix originating in the discretized linear systems of the space-fractional diffusion equations. The SHSS iterative method is employed to solve the constant coefficient space-fractional diffusion equations (1), the PCG method is used to solve the Hermitian positive definite linear systems in SHSS iteration, and two new circulant preconditioners are given to further improve the efficiency of the PCG method. Numerical experiments have been used to demonstrate that the proposed double-layer iterative method is efficient.

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