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Multilevel Circulant Preconditioner for High-Dimensional Fractional Diffusion Equations

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Abstract. High-dimensional two-sided space fractional diffusion equations with variable diffusion coefficients are discussed. The problems can be solved by an implicit finite difference scheme that is proven to be uniquely solvable, unconditionally stable and first-order convergent in the infinity norm. A nonsingular multilevel circulant preconditoner is proposed to accelerate the convergence rate of the Krylov subspace linear system solver efficiently. The preconditoned matrix for fast convergence is a sum of the identity matrix, a matrix with small norm, and a matrix with low rank under certain conditions. Moreover, the preconditioner is practical, with an O($N \log N$) operation cost and O(N) memory requirement. Illustrative numerical examples are also presented.

AMS subject classifications: 65F10, 65L12, 65T50, 26A33

Key words: High-dimensional two-sided fractional diffusion equation, implicit finite difference method, unconditionally stable, multilevel circulant preconditioner, GMRES method.

1. Introduction

Fractional diffusion equations (FDE) arise in many applications — e.g. modelling the chaotic dynamics of classical conservative systems [59], groundwater contaminant transport [2, 3], turbulent flow [5, 46], anomalous electrodiffusion in nerve cells [21], the foraging behaviour of animals [39] and the singling of biological cells [40], the design of photocopiers and laser printers [44], fluid and continuum mechanics [28], electrochemistry [35], biology [27], finance [38], image processing [1], and in physics [32, 47].

As there are very few cases of FDE where closed-form analytical solutions are available, numerical solutions for FDE have been developed intensively, including finite difference methods [20, 23, 29–31, 33, 49–51], finite element methods [15, 17, 41] and spectral methods [26, 45]. Nevertheless, since the fractional differential operator is nonlocal, most numerical methods for FDE generate dense coefficient matrices, and even full matrices in one-dimensional (1D) cases [56, 57], which usually require a computational cost of $O(N^3)$ and storage of $O(N^2)$ where N is the size of the matrix.

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Meerschaet *et al.* [29–31] proposed an implicit finite difference scheme for solving two-sided FDE, in which the shifted Grünwald-Letnikov difference approximation is employed. The difference scheme was proven to be convergent on analysing the spectral radius of the coefficient matrix of the discretised linear system, and here we show that the scheme is uniquely solvable, unconditionally stable and first-order convergent in the infinity norm. A similar result for two-dimensional (2D) FDE has been obtained in the Riesz sense [11, 24], and for two-sided FDE in the 1D case [13].

To solve the nonsymmetric linear system at each time level of the difference scheme in the 1D case, Wang *et al.* found the Toeplitz-like structure of the discrete linear system of FDE, and developed a fast method with an O(N) storage requirement and O($N\log N$) computational cost [56]. Several efficient methods using the fast Fourier transform (FFT) were then based on this Toeplitz-like structure [22, 25, 36]. In higher dimensions, an alternating-direction scheme for FDE with variable diffusion coefficients was proposed [55], and its unconditional stability and convergence was proven under certain conditions. The computational cost for solving the alternating-direction scheme is O($N \log N$) at each iteration of the Krylov subspace method, with the memory requirement O(N). On the other hand, Wang *et al.* [54, 57] proposed a Krylov subspace method to solve the discretised linear system, where (due to the block Toeplitz-like structure of the coefficient matrix) each iteration of the Krylov subspace method can be done in O($N \log N$) operations via the FFT and the memory requirement is O(N). However, the convergence rate of this Krylov subspace method is slow when the coefficient matrix is ill-conditioned, such as when the diffusion coefficients are large. In order to accelerate its convergence rate, a preconditioner is proposed in the second part of this article.

Circulant preconditioners have previously been shown to be effective for solving Toeplitz systems [7, 8, 34], and a Strang-based circulant preconditioner was developed successfully for solving 1D FDE problems [22]. For high-dimensional problems, on noting the tensor structure of the coefficient matrix a multilevel circulant preconditioner is proposed that is shown to be nonsingular. Since the multilevel circulant preconditioner can be diagonalised by a high-dimensional Fourier matrix, the product of the inverse of the preconditioner with any vector can be done in $O(N \log N)$ operations via a high-dimensional FFT. The operation cost in each iteration of the preconditioned Krylov subspace method is therefore $O(N \log N)$ with an $O(N)$ memory requirement. On the other hand, under certain conditions the preconditioned matrix is shown to be equal to a sum of the identity matrix, a matrix with small norm and a matrix with low rank. Fast convergence of the preconditioned Krylov subspace method can therefore be expected, and we undertook numerical tests to reveal the effectiveness of the multilevel circulant preconditioner. Furthermore, due to the similar structure of the coefficient matrix, the proposed multilevel circulant preconditioner can be applied to implicit finite difference schemes with high-order fractional derivative approximations [12, 48, 52, 53, 58, 60], and to FDE with a nonlinear reaction term [24].

In Section 2, an implicit finite difference discretisation for 2D two-sided FDE is analysed, where unique solvability, unconditional stability and first-order convergence in the infinity norm are shown theoretically for any nonnegative variable diffusion coefficients. A level-2 circulant preconditioner for 2D FDE is constructed in Section 3, together with the

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property of the preconditioned matrix. The theoretical results for three-dimensional (3D) problems are provided in Section 4. Numerical examples are presented in Section 5 to show the efficiency of the preconditioner and the first-order convergence of the finite difference scheme in the infinity norm, and our concluding remarks are made in Section 6.

2. 2D FDE and Finite Difference Discretisation

Let us consider the following 2D FDE problem:

$$\begin{cases} \dfrac{\partial u(x,y,t)}{\partial t} = d_+(x,y,t)\dfrac{\partial^\alpha u(x,y,t)}{\partial_+ x^\alpha} + d_-(x,y,t)\dfrac{\partial^\alpha u(x,y,t)}{\partial_- x^\alpha} \\ \qquad + e_+(x,y,t)\dfrac{\partial^\beta u(x,y,t)}{\partial_+ y^\beta} + e_-(x,y,t)\dfrac{\partial^\beta u(x,y,t)}{\partial_- y^\beta} + f(x,y,t)\,, \\ \qquad (x,y)\in\Omega\,, \qquad t\in(0,T]\,, \\ u(x,y,t) = 0\,, \qquad (x,y)\in\partial\Omega, \quad t\in(0,T]\,, \\ u(x,y,0) = u_0(x,y)\,, \qquad (x,y)\in\bar{\Omega}\,, \end{cases} \tag{2.1}$$

where $\Omega = (x_L, x_R)\times(y_L, y_R)$ is a rectangular domain, $\alpha,\beta\in(1,2)$ are the orders of the fractional derivatives, $f(x,y,t)$ is the source term, and the diffusion coefficients $d_\pm(x,y,t)$ and $e_\pm(x,y,t)$ are nonnegative. The left-sided fractional derivatives $\partial^\alpha u(x,y,t)/\partial_+ x^\alpha$ and $\partial^\beta u(x,y,t)/\partial_+ y^\beta$, and the right-sided fractional derivatives $\partial^\alpha u(x,y,t)/\partial_- x^\alpha$ and $\partial^\beta u(x,y,t)/\partial_- y^\beta$, are defined in the following Grünwald-Letnikov form [37]:

$$\begin{aligned} \frac{\partial^\alpha u(x,y,t)}{\partial_+ x^\alpha} &= \lim_{h_1\to 0^+}\frac{1}{h_1^\alpha}\sum_{k=0}^{\lfloor (x-x_L)/h_1\rfloor} g_k^{(\alpha)} u(x-kh_1,y,t)\,, \\ \frac{\partial^\beta u(x,y,t)}{\partial_+ y^\beta} &= \lim_{h_2\to 0^+}\frac{1}{h_2^\beta}\sum_{k=0}^{\lfloor (y-y_L)/h_2\rfloor} g_k^{(\beta)} u(x,y-kh_2,t)\,, \\ \frac{\partial^\alpha u(x,y,t)}{\partial_- x^\alpha} &= \lim_{h_1\to 0^+}\frac{1}{h_1^\alpha}\sum_{k=0}^{\lfloor (x_R-x)/h_1\rfloor} g_k^{(\alpha)} u(x+kh_1,y,t)\,, \\ \frac{\partial^\beta u(x,y,t)}{\partial_- y^\beta} &= \lim_{h_2\to 0^+}\frac{1}{h_2^\beta}\sum_{k=0}^{\lfloor (y_R-y)/h_2\rfloor} g_k^{(\beta)} u(x,y+kh_2,t)\,, \end{aligned}$$

where $\lfloor\cdot\rfloor$ denotes the floor function, and for all $1<\xi<2$ the sequence $\{g_k^{(\xi)}\}_k$ is defined as

$$\begin{cases} g_0^{(\xi)} = 1\,, \\ g_k^{(\xi)} = \dfrac{(-1)^k}{k!}\xi(\xi-1)\cdots(\xi-k+1)\,, \qquad k=1,2,3,\cdots\,, \end{cases}$$

which can be evaluated by the recurrence relation

$$g_{k+1}^{(\xi)} = \left(1-\frac{\xi+1}{k+1}\right)g_k^{(\xi)}\,, \qquad k=0,1,2,\cdots\,.$$

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The sequence $\{g_k^{(\xi)}\}_k$ has some useful properties [30, 31, 56], as summarised in the following proposition.

Proposition 2.1. *For all* $1 < \xi < 2$,

$$\begin{cases} g_0^{(\xi)} = 1\,, \qquad g_1^{(\xi)} = -\xi < 0\,, \qquad g_2^{(\xi)} > g_3^{(\xi)} > \cdots > 0\,, \\ \sum_{k=0}^{\infty} g_k^{(\xi)} = 0\,, \qquad \sum_{k=0}^{n} g_k^{(\xi)} < 0\,, \qquad \forall n \geq 1\,. \end{cases}$$

Let N_1, N_2 and M be positive integers; and let

$$h_1 = \frac{x_{_R} - x_{_L}}{N_{_1} + 1}\,, \qquad h_2 = \frac{y_{_R} - y_{_L}}{N_{_2} + 1}\,, \qquad \Delta t = \frac{T}{M}\,,$$

denote the sizes of the spatial grids and time step, respectively. We define the spatial and temporal partition $x_i = x_{_L} + ih_1$ for $i = 0, 1, \cdots, N_1 + 1$, $y_j = y_{_L} + jh_2$ for $j = 0, 1, \cdots, N_2 + 1$ and $t_m = m\Delta t$ for $m = 0, 1, \cdots, M$; and also write $u_{i,j}^{(m)} = u(x_i, y_j, t_m)$, $d_{\pm,i,j}^{(m)} = d_{\pm}(x_i, y_j, t_m)$, $e_{\pm,i,j}^{(m)} = e_{\pm}(x_i, y_j, t_m)$ and $f_{i,j}^{(m)} = f(x_i, y_j, t_m)$. From the shifted Grünwald approximation [30, 31]

$$\begin{aligned} \frac{\partial^{\alpha} u(x_i, y_j, t_m)}{\partial_+ x^{\alpha}} &= \frac{1}{h_1^{\alpha}} \sum_{k=0}^{i+1} g_k^{(\alpha)} u_{i-k+1,j}^{(m)} + O(h_1)\,, \\ \frac{\partial^{\beta} u(x_i, y_j, t_m)}{\partial_+ y^{\beta}} &= \frac{1}{h_2^{\beta}} \sum_{l=0}^{j+1} g_l^{(\beta)} u_{i,j-l+1}^{(m)} + O(h_2)\,, \\ \frac{\partial^{\alpha} u(x_i, y_j, t_m)}{\partial_- x^{\alpha}} &= \frac{1}{h_1^{\alpha}} \sum_{k=0}^{N_1-i+2} g_k^{(\alpha)} u_{i+k-1,j}^{(m)} + O(h_1)\,, \\ \frac{\partial^{\beta} u(x_i, y_j, t_m)}{\partial_- y^{\beta}} &= \frac{1}{h_2^{\beta}} \sum_{l=0}^{N_2-j+2} g_l^{(\beta)} u_{i,j+l-1}^{(m)} + O(h_2)\,, \end{aligned}$$

the FDE in (2.1) can be written as

$$\begin{aligned} \frac{u_{i,j}^{(m)} - u_{i,j}^{(m-1)}}{\Delta t} = &\frac{d_{+,i,j}^{(m)}}{h_1^{\alpha}} \sum_{k=0}^{i+1} g_k^{(\alpha)} u_{i-k+1,j}^{(m)} + \frac{d_{-,i,j}^{(m)}}{h_1^{\alpha}} \sum_{k=0}^{N_1-i+2} g_k^{(\alpha)} u_{i+k-1,j}^{(m)} + \frac{e_{+,i,j}^{(m)}}{h_2^{\beta}} \sum_{l=0}^{j+1} g_l^{(\beta)} u_{i,j-l+1}^{(m)} \\ &+ \frac{e_{-,i,j}^{(m)}}{h_2^{\beta}} \sum_{l=0}^{N_2-j+2} g_l^{(\beta)} u_{i,j+l-1}^{(m)} + f_{i,j}^{(m)} + R_{i,j}^{(m)}\,, \\ &1 \leq i \leq N_1\,, \quad 1 \leq j \leq N_2\,, \quad m = 1, 2, \cdots, M\,, \end{aligned} \tag{2.2}$$

where $|R_{i,j}^{(m)}| \leq C(\Delta t + h_1 + h_2)$, for some positive constant C. On neglecting the term $R_{i,j}^{(m)}$, we obtain the implicit finite difference scheme [29]

$$U_{i,j}^{(m)} - \nu_1 d_{+,i,j}^{(m)} \sum_{k=0}^{i+1} g_k^{(\alpha)} U_{i-k+1,j}^{(m)} - \nu_1 d_{-,i,j}^{(m)} \sum_{k=0}^{N_1-i+2} g_k^{(\alpha)} U_{i+k-1,j}^{(m)}$$

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$$-\nu_2 e^{(m)}_{+,i,j}\sum_{l=0}^{j+1} g^{(\beta)}_l U^{(m)}_{i,j-l+1} - \nu_2 e^{(m)}_{-,i,j}\sum_{l=0}^{N_2-j+2} g^{(\beta)}_l U^{(m)}_{i,j+l-1} = U^{(m-1)}_{i,j} + f^{(m)}_{i,j}\,,$$
$$1 \le i \le N_1\,, \quad 1 \le j \le N_2\,, \quad m = 1,2,\cdots,M\,, \tag{2.3}$$

where

$$\nu_1 = \frac{\Delta t}{h_1^\alpha} \quad \text{and} \quad \nu_2 = \frac{\Delta t}{h_2^\beta}\,.$$

Theorem 2.1. *The implicit finite difference scheme* (2.3) *for solving 2D two-sided FDE with nonnegative variable diffusion coefficients is uniquely solvable.*

Proof. The result follows from the fact that the coefficient matrix of the implicit finite difference scheme is nonsingular — cf. Lemma 2.1 in Section 2.3 below. □

2.1. Unconditional stability

The unconditional stability of the above finite difference scheme is studied in [29–31] through analysing the spectral radius of the coefficient matrix of the scheme. We now prove the unconditional stability for all nonnegative variable diffusion coefficients in terms of the infinity norm. For all $i = 1,2,\cdots,N_1$, $j = 1,2,\cdots,N_2$ and $m = 1,2,\cdots,M$, let $\tilde{U}^{(m)}_{i,j}$ and $U^{(m)}_{i,j}$ be two solutions of the difference scheme (2.3), and define $\epsilon^{(m)}_{i,j} = \tilde{U}^{(m)}_{i,j} - U^{(m)}_{i,j}$. Then $\epsilon^{(m)}_{i,j}$ satisfies the equation

$$\epsilon^{(m)}_{i,j} - \nu_1 d^{(m)}_{+,i,j}\sum_{k=0}^{i+1} g^{(\alpha)}_k \epsilon^{(m)}_{i-k+1,j} - \nu_1 d^{(m)}_{-,i,j}\sum_{k=0}^{N_1-i+2} g^{(\alpha)}_k \epsilon^{(m)}_{i+k-1,j}$$
$$-\nu_2 e^{(m)}_{+,i,j}\sum_{l=0}^{j+1} g^{(\beta)}_l \epsilon^{(m)}_{i,j-l+1} - \nu_2 e^{(m)}_{-,i,j}\sum_{l=0}^{N_2-j+2} g^{(\beta)}_l \epsilon^{(m)}_{i,j+l-1} = \epsilon^{(m-1)}_{i,j}\,,$$
$$1 \le i \le N_1\,, \quad 1 \le j \le N_2\,, \quad m = 1,2,\cdots,M\,. \tag{2.4}$$

Denoting $\mathbf{E}^{(m)} = (\epsilon^{(m)}_{1,1}, \epsilon^{(m)}_{2,1}, \cdots, \epsilon^{(m)}_{N_1,1}, \epsilon^{(m)}_{1,2}, \cdots, \epsilon^{(m)}_{N_1,2}, \cdots, \epsilon^{(m)}_{N_1,N_2})^T$, we now prove the unconditional stability in the sense that

$$\|\mathbf{E}^{(m)}\|_\infty \le \|\mathbf{E}^{(0)}\|_\infty\,, \qquad \forall\, m = 1,2,\cdots,M\,.$$

Theorem 2.2. *The implicit finite difference scheme* (2.3) *for solving 2D two-sided FDE with nonnegative variable diffusion coefficients is unconditionally stable.*

Proof. Assume that $\|\mathbf{E}^{(m)}\|_\infty = |\epsilon^{(m)}_{i_0,j_0}|$ for some $1 \le i_0 \le N_1$ and $1 \le j_0 \le N_2$. Then using Proposition 2.1 and the triangle inequality, we have

$$\|\mathbf{E}^{(m)}\|_\infty = |\epsilon^{(m)}_{i_0,j_0}| \le |\epsilon^{(m)}_{i_0,j_0}| - \nu_1 d^{(m)}_{+,i_0,j_0}\sum_{k=0}^{i_0+1} g^{(\alpha)}_k |\epsilon^{(m)}_{i_0,j_0}| - \nu_1 d^{(m)}_{-,i_0,j_0}\sum_{k=0}^{N_1-i_0+2} g^{(\alpha)}_k |\epsilon^{(m)}_{i_0,j_0}|$$

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$$
\begin{aligned}
&- \nu_2 e^{(m)}_{+,i_0,j_0} \sum_{l=0}^{j_0+1} g^{(\beta)}_l |\epsilon^{(m)}_{i_0,j_0}| - \nu_2 e^{(m)}_{-,i_0,j_0} \sum_{l=0}^{N_2-j_0+2} g^{(\beta)}_l |\epsilon^{(m)}_{i_0,j_0}| \\
=&|\epsilon^{(m)}_{i_0,j_0}| - \nu_1 (d^{(m)}_{+,i_0,j_0} + d^{(m)}_{-,i_0,j_0}) g^{(\alpha)}_1 |\epsilon^{(m)}_{i_0,j_0}| - \nu_2 (e^{(m)}_{+,i_0,j_0} + e^{(m)}_{-,i_0,j_0}) g^{(\beta)}_1 |\epsilon^{(m)}_{i_0,j_0}| \\
&- \nu_1 d^{(m)}_{+,i_0,j_0} \sum_{k=0,k\neq 1}^{i_0+1} g^{(\alpha)}_k |\epsilon^{(m)}_{i_0,j_0}| - \nu_1 d^{(m)}_{-,i_0,j_0} \sum_{k=0,k\neq 1}^{N_1-i_0+2} g^{(\alpha)}_k |\epsilon^{(m)}_{i_0,j_0}| \\
&- \nu_2 e^{(m)}_{+,i_0,j_0} \sum_{l=0,l\neq 1}^{j_0+1} g^{(\beta)}_l |\epsilon^{(m)}_{i_0,j_0}| - \nu_2 e^{(m)}_{-,i_0,j_0} \sum_{l=0,l\neq 1}^{N_2-j_0+2} g^{(\beta)}_l |\epsilon^{(m)}_{i_0,j_0}| \\
\le&\Big[1 - \nu_1 (d^{(m)}_{+,i_0,j_0} + d^{(m)}_{-,i_0,j_0}) g^{(\alpha)}_1 - \nu_2 (e^{(m)}_{+,i_0,j_0} + e^{(m)}_{-,i_0,j_0}) g^{(\beta)}_1\Big] |\epsilon^{(m)}_{i_0,j_0}| \\
&- \nu_1 d^{(m)}_{+,i_0,j_0} \sum_{k=0,k\neq 1}^{i_0+1} g^{(\alpha)}_k |\epsilon^{(m)}_{i_0-k+1,j_0}| - \nu_1 d^{(m)}_{-,i_0,j_0} \sum_{k=0,k\neq 1}^{N_1-i_0+2} g^{(\alpha)}_k |\epsilon^{(m)}_{i_0+k-1,j_0}| \\
&- \nu_2 e^{(m)}_{+,i_0,j_0} \sum_{l=0,l\neq 1}^{j_0+1} g^{(\beta)}_l |\epsilon^{(m)}_{i_0,j_0-l+1}| - \nu_2 e^{(m)}_{-,i_0,j_0} \sum_{l=0,l\neq 1}^{N_2-j_0+2} g^{(\beta)}_l |\epsilon^{(m)}_{i_0,j_0+l-1}| \\
\le&\left|\Big[1 - \nu_1 (d^{(m)}_{+,i_0,j_0} + d^{(m)}_{-,i_0,j_0}) g^{(\alpha)}_1 - \nu_2 (e^{(m)}_{+,i_0,j_0} + e^{(m)}_{-,i_0,j_0}) g^{(\beta)}_1\Big] \epsilon^{(m)}_{i_0,j_0}\right| \\
&- \left|\nu_1 d^{(m)}_{+,i_0,j_0} \sum_{k=0,k\neq 1}^{i_0+1} g^{(\alpha)}_k \epsilon^{(m)}_{i_0-k+1,j_0}\right| - \left|\nu_1 d^{(m)}_{-,i_0,j_0} \sum_{k=0,k\neq 1}^{N_1-i_0+2} g^{(\alpha)}_k \epsilon^{(m)}_{i_0+k-1,j_0}\right| \\
&- \left|\nu_2 e^{(m)}_{+,i_0,j_0} \sum_{l=0,l\neq 1}^{j_0+1} g^{(\beta)}_l \epsilon^{(m)}_{i_0,j_0-l+1}\right| - \left|\nu_2 e^{(m)}_{-,i_0,j_0} \sum_{l=0,l\neq 1}^{N_2-j_0+2} g^{(\beta)}_l \epsilon^{(m)}_{i_0,j_0+l-1}\right| \\
\le&\left|\epsilon^{(m)}_{i_0,j_0} - \nu_1 d^{(m)}_{+,i_0,j_0} \sum_{k=0}^{i_0+1} g^{(\alpha)}_k \epsilon^{(m)}_{i_0-k+1,j_0} - \nu_1 d^{(m)}_{-,i_0,j_0} \sum_{k=0}^{N_1-i_0+2} g^{(\alpha)}_k \epsilon^{(m)}_{i_0+k-1,j_0}\right. \\
&\left. - \nu_2 e^{(m)}_{+,i_0,j_0} \sum_{l=0}^{j_0+1} g^{(\beta)}_l \epsilon^{(m)}_{i_0,j_0-l+1} - \nu_2 e^{(m)}_{-,i_0,j_0} \sum_{l=0}^{N_2-j_0+2} g^{(\beta)}_l \epsilon^{(m)}_{i_0,j_0+l-1}\right| \\
=&|\epsilon^{(m-1)}_{i_0,j_0}| \le \|\mathbf{E}^{(m-1)}\|_\infty ,
\end{aligned}
$$

where the last equality follows from (2.4). □

2.2. First-order convergence in the infinity norm

Theorem 2.3. *If $U^{(m)}_{i,j}$ denotes the numerical solution for $u^{(m)}_{i,j}$ computed using the implicit difference scheme* (2.3)*, then there is a positive constant C' such that*

$$\left|u^{(m)}_{i,j} - U^{(m)}_{i,j}\right| \le C'(\Delta t + h_1 + h_2)$$

for all $i = 0, 1, \cdots, N_1$, $j = 0, 1, \cdots, N_2$, $m = 0, 1, \cdots, M$.

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Proof. Let $\varepsilon_{i,j}^{(m)} = u_{i,j}^{(m)} - U_{i,j}^{(m)}$ and $R_{\max} = \max_{0\le i\le N_1,\,0\le j\le N_2,\,0\le m\le M}|R_{i,j}^{(m)}|$. From (2.2) and (2.3), $\varepsilon_{i,j}^{(m)}$ satisfies the perturbation equation

$$\begin{aligned}
&\varepsilon_{i,j}^{(m)} - \nu_1 d_{+,i,j}^{(m)} \sum_{k=0}^{i+1} g_k^{(\alpha)} \varepsilon_{i-k+1,j}^{(m)} - \nu_1 d_{-,i,j}^{(m)} \sum_{k=0}^{N_1-i+2} g_k^{(\alpha)} \varepsilon_{i+k-1,j}^{(m)} \\
&\quad - \nu_2 e_{+,i,j}^{(m)} \sum_{l=0}^{j+1} g_l^{(\beta)} \varepsilon_{i,j-l+1}^{(m)} - \nu_2 e_{-,i,j}^{(m)} \sum_{l=0}^{N_2-j+2} g_l^{(\beta)} \varepsilon_{i,j+l-1}^{(m)} = \varepsilon_{i,j}^{(m-1)} + \Delta t R_{i,j}^{(m)}\,, \\
&\qquad 1 \le i \le N_1\,, \quad 1 \le j \le N_2\,, \quad m = 1, 2, \cdots, M\,. \qquad (2.5)
\end{aligned}$$

Denoting

$$\widetilde{\mathbf{E}}^{(m)} = \left(\varepsilon_{1,1}^{(m)}, \varepsilon_{2,1}^{(m)}, \cdots, \varepsilon_{N_1,1}^{(m)}, \varepsilon_{1,2}^{(m)}, \cdots, \varepsilon_{N_1,2}^{(m)}, \cdots, \varepsilon_{N_1,N_2}^{(m)}\right)^T,$$

and assuming that $\|\widetilde{\mathbf{E}}^{(m)}\|_\infty = |\varepsilon_{i_0,j_0}^{(m)}|$, by using the same technique in the proof of the unconditional stability and (2.5) we get

$$\begin{aligned}
\|\widetilde{\mathbf{E}}^{(m)}\|_\infty = |\varepsilon_{i_0,j_0}^{(m)}| &\le \Bigg| \varepsilon_{i_0,j_0}^{(m)} - \nu_1 d_{+,i_0,j_0}^{(m)} \sum_{k=0}^{i_0+1} g_k^{(\alpha)} \varepsilon_{i_0-k+1,j_0}^{(m)} - \nu_1 d_{-,i_0,j_0}^{(m)} \sum_{k=0}^{N_1-i_0+2} g_k^{(\alpha)} \varepsilon_{i_0+k-1,j_0}^{(m)} \\
&\quad - \nu_2 e_{+,i_0,j_0}^{(m)} \sum_{l=0}^{j_0+1} g_l^{(\beta)} \varepsilon_{i_0,j_0-l+1}^{(m)} - \nu_2 e_{-,i_0,j_0}^{(m)} \sum_{l=0}^{N_2-j_0+2} g_l^{(\beta)} \varepsilon_{i_0,j_0+l-1}^{(m)} \Bigg| \\
&= \left| \varepsilon_{i_0,j_0}^{(m-1)} + \Delta t R_{i_0,j_0}^{(m)} \right| \le \|\widetilde{\mathbf{E}}^{(m-1)}\|_\infty + \Delta t R_{\max} \le M \Delta t R_{\max} \\
&\le C'(\Delta t + h_1 + h_2)\,,
\end{aligned}$$

where C' is a positive constant. □

Remark 2.1. For d-dimensional ($d \ge 3$) FDE problems, similar proofs can be established for the unique solvability, unconditional stability and the first-order convergence of the implicit finite difference scheme.

2.3. Matrix form and linear system solver

Let $\mathscr{I}_N$ be the $N \times N$ identity matrix, and

$$\begin{aligned}
\mathbf{u}^{(m)} &= \left(U_{1,1}^{(m)}, \cdots, U_{N_1,1}^{(m)}, U_{1,2}^{(m)}, \cdots, U_{N_1,2}^{(m)}, \cdots, U_{1,N_2}^{(m)}, \cdots, U_{N_1,N_2}^{(m)}\right)^T, \\
\mathbf{f}^{(m)} &= \left(f_{1,1}^{(m)}, \cdots, f_{N_1,1}^{(m)}, f_{1,2}^{(m)}, \cdots, f_{N_1,2}^{(m)}, \cdots, f_{1,N_2}^{(m)}, \cdots, f_{N_1,N_2}^{(m)}\right)^T, \\
\mathbf{d}_\pm^{(m)} &= \left(d_{\pm,1,1}^{(m)}, \cdots, d_{\pm,N_1,1}^{(m)}, d_{\pm,1,2}^{(m)}, \cdots, d_{\pm,N_1,2}^{(m)}, \cdots, d_{\pm,1,N_2}^{(m)}, \cdots, d_{\pm,N_1,N_2}^{(m)}\right)^T, \\
\mathbf{e}_\pm^{(m)} &= \left(e_{\pm,1,1}^{(m)}, \cdots, e_{\pm,N_1,1}^{(m)}, e_{\pm,1,2}^{(m)}, \cdots, e_{\pm,N_1,2}^{(m)}, \cdots, e_{\pm,1,N_2}^{(m)}, \cdots, e_{\pm,N_1,N_2}^{(m)}\right)^T.
\end{aligned}$$

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The numerical scheme (2.3) can be written in the following matrix form:

$$(\mathscr{I}_{N_1N_2} - \mathscr{A}_x^{(m)} - \mathscr{A}_y^{(m)})\mathbf{u}^{(m)} = \mathbf{u}^{(m-1)} + \Delta t \mathbf{f}^{(m)}, \tag{2.6}$$

where

$$\mathscr{A}_x^{(m)} = \nu_1 \mathrm{diag}(\mathbf{d}_+^{(m)})(\mathscr{I}_{N_2} \otimes \mathscr{G}_\alpha) + \nu_1 \mathrm{diag}(\mathbf{d}_-^{(m)})(\mathscr{I}_{N_2} \otimes \mathscr{G}_\alpha^T),$$
$$\mathscr{A}_y^{(m)} = \nu_2 \mathrm{diag}(\mathbf{e}_+^{(m)})(\mathscr{G}_\beta \otimes \mathscr{I}_{N_1}) + \nu_2 \mathrm{diag}(\mathbf{e}_-^{(m)})(\mathscr{G}_\beta^T \otimes \mathscr{I}_{N_1}).$$

Here diag($\mathbf{v}$) denotes the diagonal matrix with diagonal $\mathbf{v}$ and $\otimes$ the Kronecker product, and the matrix

$$\mathscr{G}_\xi = \begin{pmatrix} g_1^{(\xi)} & g_0^{(\xi)} & 0 & \cdots & 0 & 0 \\ g_2^{(\xi)} & g_1^{(\xi)} & g_0^{(\xi)} & 0 & \ddots & 0 \\ \vdots & g_2^{(\xi)} & g_1^{(\xi)} & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & 0 \\ g_{N_i-1}^{(\xi)} & \ddots & \ddots & \ddots & g_1^{(\xi)} & g_0^{(\xi)} \\ g_{N_i}^{(\xi)} & g_{N_i-1}^{(\xi)} & \cdots & \cdots & g_2^{(\xi)} & g_1^{(\xi)} \end{pmatrix}, \quad (\xi, i) = (\alpha, 1) \text{ or } (\beta, 2),$$

is Toeplitz. The following lemma gives the invertibility of the coefficient matrix of (2.6).

Lemma 2.1. *The coefficient matrix*

$$\mathscr{M}^{(m)} = \mathscr{I}_{N_1N_2} - \mathscr{A}_x^{(m)} - \mathscr{A}_y^{(m)} \tag{2.7}$$

of the linear system (2.6) *is nonsingular.*

Proof. Given the Proposition 2.1, one can prove that the Toeplitz matrices $\mathscr{G}_\xi$ and $\mathscr{G}_\xi^T$ are strictly diagonally dominant with negative elements in the main diagonal. Consequently, for any positive definite diagonal matrix $\mathscr{D}$ the matrices $\mathscr{D}(\mathscr{I} \otimes \mathscr{G}_\xi)$, $\mathscr{D}(\mathscr{I} \otimes \mathscr{G}_\xi^T)$, $\mathscr{D}(\mathscr{G}_\xi \otimes \mathscr{I})$, and $\mathscr{D}(\mathscr{G}_\xi^T \otimes \mathscr{I})$ are also strictly diagonally dominant with negative elements in the main diagonal. From the Geršhgorin circle theorem, the real parts of all eigenvalues of the matrix $\mathscr{A}_x^{(m)} + \mathscr{A}_y^{(m)}$ are therefore negative, so $\mathscr{M}^{(m)}$ is nonsingular.

It is notable that the matrix $\mathscr{M}^{(m)}$ is nonsymmetric except for the case where $d_\pm$, $e_\pm$ are constants with $d_+ = d_-$, $e_+ = e_-$ and $N_1 = N_2$, where N_1 and N_2 are the number of interior mesh points in the x- and y-directions, respectively. If a direct method is used to solve the linear system (2.6), it requires $O(N_1^3 N_2^3)$ operations and $O(N_1^2 N_2^2)$ memory. Nevertheless, as $\mathscr{M}^{(m)}$ possesses block Toeplitz-like structure, Wang [57] proposed to solve (2.6) using the Krylov subspace method where the complexity in each iteration is $O(N_1N_2 \log N_1N_2)$ and the memory requirement is $O(N_1N_2)$. However, the coefficient matrix $\mathscr{M}^{(m)}$ could be ill-conditioned such that the iterative linear system solver converges slowly. In the following section, a preconditioner is proposed to accelerate the convergence rate of the Krylov subspace method.

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3. Level-2 Circulant Preconditioner

3.1. Definition of the level-2 circulant preconditioner

A Toeplitz matrix

$$\mathscr{P} = \begin{pmatrix} p_0 & p_{-1} & \cdots & p_{2-N} & p_{1-N} \\ p_1 & p_0 & p_{-1} & \ddots & p_{2-N} \\ \vdots & p_1 & p_0 & \ddots & \vdots \\ p_{N-2} & \ddots & \ddots & \ddots & p_{-1} \\ p_{N-1} & p_{N-2} & \cdots & p_1 & p_0 \end{pmatrix}_{N\times N}$$

is said to possess circulant structure if

$$p_k = p_{k-N}, \quad \text{for all } k = 1, \cdots, N-1.$$

In solving the Toeplitz system $\mathscr{P}\mathbf{u} = \mathbf{b}$ using the Krylov subspace method, it is well-known that the convergence rate can be accelerated by applying circulant preconditioners [7]. One famous choice is Strang's circulant preconditioner $s(\mathscr{P})$ [9], where the circulant matrix $s(\mathscr{P})$ can be obtained by copying the central diagonals of $\mathscr{P}$ to complete the circulant requirement [8, 18]. Thus the entries in the first column $(s_0, s_1, \cdots, s_{N-1})^T$ of $s(\mathscr{P})$ are given by

$$s_j = \begin{cases} p_j\,, & 0 \le j \le N/2-1\,, \\ 0\,, & j = N/2\,, \ \text{if } N \text{ is even}\,, \\ p_{j-N}\,, & N/2 < j \le N-1\,. \end{cases}$$

Then we solve (2.6) by solving the equivalent preconditioned system

$$(\mathscr{S}_2^{(m)})^{-1}\mathscr{M}^{(m)}\mathbf{u}^{(m)} = (\mathscr{S}_2^{(m)})^{-1}\left(\mathbf{u}^{(m-1)} + \Delta t\mathbf{f}^{(m)}\right), \tag{3.1}$$

with the proposed Strang-based level-2 circulant preconditioner $\mathscr{S}_2^{(m)}$ defined as

$$\begin{aligned}\mathscr{S}_2^{(m)} =& \mathscr{I}_{N_1N_2} - \mathscr{I}_{N_2} \otimes \nu_1\left[\bar{d}_+^{(m)} s(\mathscr{G}_\alpha) + \bar{d}_-^{(m)} s(\mathscr{G}_\alpha^T)\right] \\ & - \nu_2[\bar{e}_+^{(m)} s(\mathscr{G}_\beta) + \bar{e}_-^{(m)} s(\mathscr{G}_\beta^T)] \otimes \mathscr{I}_{N_1}\,,\end{aligned}$$

where

$$\bar{d}_\pm^{(m)} = \frac{1}{N_1N_2}\sum_{i=1}^{N_1}\sum_{j=1}^{N_2} d_{\pm,i,j}^{(m)} \quad \text{and} \quad \bar{e}_\pm^{(m)} = \frac{1}{N_1N_2}\sum_{i=1}^{N_1}\sum_{j=1}^{N_2} e_{\pm,i,j}^{(m)}$$

are the respective averages of the diffusion coefficient functions $d_\pm(x, y, t_m)$ and $e_\pm(x, y, t_m)$ over all interior spatial grid points. The level-2 circulant preconditioner is a block circulant matrix with circulant blocks that is usually employed to precondition block Toeplitz matrices with Toeplitz blocks [6, 19].

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3.2. Basic properties of $\mathscr{S}_2^{(m)}$

Theorem 3.1. *The level-2 circulant preconditioner $\mathscr{S}_2^{(m)}$ is nonsingular.*

Proof. Since any circulant matrix is diagonalisable by a Fourier matrix $\mathscr{F}$ [14], we have

$$s(\mathscr{G}_\alpha) = \mathscr{F}_{N_1}^* \Lambda_\alpha \mathscr{F}_{N_1} \quad \text{and} \quad s(\mathscr{G}_\beta) = \mathscr{F}_{N_2}^* \Lambda_\beta \mathscr{F}_{N_2},$$

where Λ_α and Λ_β are diagonal matrices. Thus we have

$$s(\mathscr{G}_\alpha^T) = \mathscr{F}_{N_1}^* \bar{\Lambda}_\alpha \mathscr{F}_{N_1} \quad \text{and} \quad s(\mathscr{G}_\beta^T) = \mathscr{F}_{N_2}^* \bar{\Lambda}_\beta \mathscr{F}_{N_2},$$

where $\bar{\Lambda}_\alpha$ and $\bar{\Lambda}_\beta$ are the respective complex conjugates of Λ_α and Λ_β such that

$$\mathscr{S}_2^{(m)} = (\mathscr{F}_{N_2} \otimes \mathscr{F}_{N_1})^* \Lambda_{s_2}^{(m)} (\mathscr{F}_{N_2} \otimes \mathscr{F}_{N_1}),$$

where

$$\Lambda_{s_2}^{(m)} = \mathscr{I}_{N_1 N_2} - \mathscr{I}_{N_2} \otimes \nu_1 (\bar{d}_+^{(m)} \Lambda_\alpha + \bar{d}_-^{(m)} \bar{\Lambda}_\alpha) - \nu_2 (\bar{e}_+^{(m)} \Lambda_\beta + \bar{e}_-^{(m)} \bar{\Lambda}_\beta) \otimes \mathscr{I}_{N_1}.$$

From [22, 42] we have $\mathrm{Re}([\Lambda_\alpha]_{i,i}) < 0$ and $\mathrm{Re}([\Lambda_\beta]_{j,j}) < 0$ for each $i = 1, \cdots, N_1$ and $j = 1, \cdots, N_2$, so $\Lambda_{s_2}^{(m)}$ is nonsingular and hence $\mathscr{S}_2^{(m)}$ is nonsingular.

Remark 3.1. $\Lambda_\alpha = \mathrm{diag}(\mathscr{F}_{N_1} \mathbf{s}_1)$ and $\Lambda_\beta = \mathrm{diag}(\mathscr{F}_{N_2} \mathbf{s}_2)$, where

$$\mathbf{s}_1 = \left(g_1^{(\alpha)}, \cdots, g_{\lfloor \frac{N_1+1}{2} \rfloor}^{(\alpha)}, 0, \cdots, 0, g_0^{(\alpha)} \right)^T \quad \text{and} \quad \mathbf{s}_2 = \left(g_1^{(\beta)}, \cdots, g_{\lfloor \frac{N_2+1}{2} \rfloor}^{(\beta)}, 0, \cdots, 0, g_0^{(\beta)} \right)^T \tag{3.2}$$

are the first columns of $s(\mathscr{G}_\alpha)$ and $s(\mathscr{G}_\beta)$, respectively.

From Theorem 3.1 and Remark 3.1, we have the following lemma.

Lemma 3.1. *For any vector* $\mathbf{v}$*, the matrix-vector product*

$$\left(\mathscr{S}_2^{(m)}\right)^{-1} \mathbf{v} = (\mathscr{F}_{N_2} \otimes \mathscr{F}_{N_1})^* \left(\Lambda_{s_2}^{(m)}\right)^{-1} (\mathscr{F}_{N_2} \otimes \mathscr{F}_{N_1}) \mathbf{v}$$

can be computed in $O(N_1 N_2 \log N_1 N_2)$ operations using the 2D FFT.

A MATLAB code to compute the product $(\mathscr{S}_2^{(m)})^{-1}\mathbf{v}$, for $N_1 = N_2 = N$ is as follows, where $\mathbf{d}$ is the diagonal vector of $\Lambda_{s_2}^{(m)}$:

```
% Computes z = S2^(-1)*v
z = fft2(reshape(v,N,N));
z = reshape(z,N^2,1)./d;
z = ifft2(reshape(z,N,N));
z = reshape(z,N^2,1);
```

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It is notable that the vector $\mathbf{d}$ is computed once in each time level, and the following is a MATLAB code to compute $\mathbf{d}$ for $N_1 = N_2 = N$, with vectors $\mathbf{s}_1$ and $\mathbf{s}_2$ given in (3.2):

```
% Computes the vector d
Lam1 = fft(s1); Lam2 = fft(s2); I = ones(N,1);
A = nu1*(d1*Lam1+d2*conj(Lam1));
B = nu2*(e1*Lam2+e2*conj(Lam2));
d = 1 - kron(I,A) - kron(B,I);
```

From Lemma 3.1 and the above computer codes, in employing the level-2 circulant preconditioner we note that the operation cost is very low and the additional code is very simple.

We end this subsection by giving a uniform bound on the spectral norm of the inverse of the preconditioner.

Lemma 3.2. *The matrix spectral norm of* $(\mathscr{S}_2^{(m)})^{-1}$ *is uniformly bounded by 1 — i.e.*

$$\left\|(\mathscr{S}_2^{(m)})^{-1}\right\|_2 \le 1\,.$$

Proof. Let $\mathrm{Re}(z)$ denote the real part of z. Since $\nu_1, \nu_2, \bar{d}_\pm^{(m)}, \bar{e}_\pm^{(m)} > 0$,

$$\begin{aligned}\left|\left(\Lambda_{s_2}^{(m)}\right)_{k,k}\right| &\ge \mathrm{Re}\left(\left(\Lambda_{s_2}^{(m)}\right)_{k,k}\right)\\ &= 1-\left(\mathscr{I}_{N_2}\otimes \nu_1\left(\bar{d}_+^{(m)}\mathrm{Re}(\Lambda_\alpha)+\bar{d}_-^{(m)}\mathrm{Re}(\bar{\Lambda}_\alpha)\right)\right)_{k,k}\\ &\quad -\left(\nu_2\left(\bar{e}_+^{(m)}\mathrm{Re}(\Lambda_\beta)+\bar{e}_-^{(m)}\mathrm{Re}(\bar{\Lambda}_\beta)\right)\otimes \mathscr{I}_{N_1}\right)_{k,k} \ge 1\end{aligned}$$

for all $k = 1, \cdots, N_1N_2$, hence

$$\left\|(\mathscr{S}_2^{(m)})^{-1}\right\|_2 = \frac{1}{\min\limits_{1\le k\le N_1N_2}\left|\left(\Lambda_{s_2}^{(m)}\right)_{k,k}\right|} \le 1\,. \quad \square$$

3.3. Fast convergence of the preconditioned Krylov subspace method

Usually, the convergence rate of the Krylov subspace method is fast if the spectrum of the preconditioned matrix is away from zero, and the preconditioned matrix can be expressed as a sum of the identity matrix, a matrix with low rank, and a matrix with small norm — this is especially true when the matrix is close to normal [4]. Let us now assume that the diffusion coefficients are independent of the space variables x and y — i.e.

$$d_{\pm,i,j}^{(m)} = d_\pm^{(m)}, \quad e_{\pm,i,j}^{(m)} = e_\pm^{(m)}, \quad \forall i = 1,\cdots,N_1\,, \quad j = 1,\cdots,N_2\,, \tag{3.3}$$

in each time level. In the following, we prove that the preconditioned matrix $(\mathscr{S}_2^{(m)})^{-1}\mathscr{M}^{(m)}$ can be expressed as a sum of the identity matrix, a matrix with small norm, and a matrix

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with rank $O(N_1+N_2)$. Throughout this section, we add a subscript to each matrix to denote the matrix size — e.g. the coefficient matrix in (2.7) now is denoted by $\mathscr{M}^{(m)}_{N_1N_2}$. Under the condition (3.3), the matrix $\mathscr{M}^{(m)}_{N_1N_2}$ now can be written as

$$\mathscr{M}^{(m)}_{N_1N_2} = \mathscr{I}_{N_1N_2} - \mathscr{I}_{N_2} \otimes \nu_1 \mathscr{A}^{(m)}_{N_1} - \nu_2 \mathscr{B}^{(m)}_{N_2} \otimes \mathscr{I}_{N_1} ,$$

where

$$\mathscr{A}^{(m)}_{N_1} = d^{(m)}_{+}\mathscr{G}_{\alpha} + d^{(m)}_{-}\mathscr{G}^{T}_{\alpha} \quad \text{and} \quad \mathscr{B}^{(m)}_{N_2} = e^{(m)}_{+}\mathscr{G}_{\beta} + e^{(m)}_{-}\mathscr{G}^{T}_{\beta}$$

are Toeplitz matrices.

Theorem 3.2. *Under the assumption* (3.3) *and* $\nu_1, \nu_2 \le \nu$, *for any* $\epsilon > 0$, *there exist* N_1' *and* N_2', *such that for all* $N_1 > N_1'$ *and* $N_2 > N_2'$ *we have*

$$(\mathscr{S}^{(m)}_2)^{-1}\mathscr{M}^{(m)}_{N_1N_2} = \mathscr{I}_{N_1N_2} + \mathscr{U}^{(m)}_{N_1N_2} + \mathscr{V}^{(m)}_{N_1N_2} ,$$

where

$$\mathrm{rank}(\mathscr{U}^{(m)}_{N_1N_2}) = O(N_1+N_2) \quad \textit{and} \quad ||\mathscr{V}^{(m)}_{N_1N_2}||_2 < \epsilon .$$

Proof. Firstly, we note

$$\mathscr{S}^{(m)}_2 - \mathscr{M}^{(m)}_{N_1N_2} = \nu_1\mathscr{I}_{N_2} \otimes \left(\mathscr{A}^{(m)}_{N_1} - s(\mathscr{A}^{(m)}_{N_1})\right) + \nu_2\left(\mathscr{B}^{(m)}_{N_2} - s(\mathscr{B}^{(m)}_{N_2})\right) \otimes \mathscr{I}_{N_1} .$$

From Lemma 5 in Ref. [22], for any $\epsilon > 0$ there exist N_1', $N_2' > 0$ such that for all $N_1 > N_1'$ and $N_2 > N_2'$ we have

$$\mathscr{A}^{(m)}_{N_1} - s(\mathscr{A}^{(m)}_{N_1}) = \widetilde{\mathscr{U}}^{(m)}_{N_1} + \widetilde{\mathscr{V}}^{(m)}_{N_1}, \qquad \mathscr{B}^{(m)}_{N_2} - s(\mathscr{B}^{(m)}_{N_2}) = \widehat{\mathscr{U}}^{(m)}_{N_2} + \widehat{\mathscr{V}}^{(m)}_{N_2}$$

where

$$\mathrm{rank}(\widetilde{\mathscr{U}}^{(m)}_{N_1}) \le C_1(\epsilon), \quad \mathrm{rank}(\widehat{\mathscr{U}}^{(m)}_{N_2}) \le C_2(\epsilon)$$

and

$$||\widetilde{\mathscr{V}}^{(m)}_{N_1}||_2 < \epsilon/2\nu , \quad ||\widehat{\mathscr{V}}^{(m)}_{N_2}||_2 < \epsilon/2\nu .$$

Here $C_1(\epsilon)$ and $C_2(\epsilon)$ are constants independent of N_1 and N_2. Now letting

$$\bar{\mathscr{U}}^{(m)}_{N_1N_2} = \nu_1\mathscr{I}_{N_2} \otimes \widetilde{\mathscr{U}}^{(m)}_{N_1} + \widehat{\mathscr{U}}^{(m)}_{N_2} \otimes \nu_2\mathscr{I}_{N_1} \qquad \bar{\mathscr{V}}^{(m)}_{N_1N_2} = \nu_1\mathscr{I}_{N_2} \otimes \widetilde{\mathscr{V}}^{(m)}_{N_1} + \widehat{\mathscr{V}}^{(m)}_{N_2} \otimes \nu_2\mathscr{I}_{N_1}$$

we have

$$\mathscr{S}^{(m)}_2 - \mathscr{M}^{(m)}_{N_1N_2} = \bar{\mathscr{U}}^{(m)}_{N_1N_2} + \bar{\mathscr{V}}^{(m)}_{N_1N_2} \tag{3.4}$$

with

$$\begin{aligned}\mathrm{rank}(\bar{\mathscr{U}}^{(m)}_{N_1N_2}) \le& \mathrm{rank}(\nu_1\mathscr{I}_{N_2} \otimes \widetilde{\mathscr{U}}_{N_1}) + \mathrm{rank}(\widehat{\mathscr{U}}_{N_2} \otimes \nu_2\mathscr{I}_{N_1}) \\ =& \mathrm{rank}(\mathscr{I}_{N_2}) \cdot \mathrm{rank}(\widetilde{\mathscr{U}}^{(m)}_{N_1}) + \mathrm{rank}(\widehat{\mathscr{U}}^{(m)}_{N_2}) \cdot \mathrm{rank}(\mathscr{I}_{N_1}) \\ \le& C_1(\epsilon)N_2 + C_2(\epsilon)N_1\end{aligned}$$

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and

$$\begin{aligned}||\bar{\mathscr{V}}^{(m)}_{N_1N_2}||_2 \leq& ||\,\nu_1\mathscr{I}_{N_2}\otimes\widetilde{\mathscr{V}}^{(m)}_{N_1}||_2 + ||\widehat{\mathscr{V}}^{(m)}_{N_2}\otimes\nu_2\mathscr{I}_{N_1}||_2\\ =&\nu_1||\widetilde{\mathscr{V}}^{(m)}_{N_1}||_2+\nu_2||\widehat{\mathscr{V}}^{(m)}_{N_2}||_2\\ <&\frac{\nu_1+\nu_2}{2\nu}\epsilon\\ <&\epsilon\,.\end{aligned}$$

By multiplying $(\mathscr{S}^{(m)}_2)^{-1}$ on both sides of (3.4), we then have

$$(\mathscr{S}^{(m)}_2)^{-1}\mathscr{M}^{(m)}_{N_1N_2}=\mathscr{I}_{N_1N_2}+\mathscr{U}^{(m)}_{N_1N_2}+\mathscr{V}^{(m)}_{N_1N_2}\,,$$

where

$$\operatorname{rank}(\mathscr{U}^{(m)}_{N_1N_2})=\operatorname{rank}\Big((\mathscr{S}^{(m)}_2)^{-1}\bar{\mathscr{U}}^{(m)}_{N_1N_2}\Big)\leq\operatorname{rank}(\bar{\mathscr{U}}^{(m)}_{N_1N_2})\leq C_1(\epsilon)N_2+C_2(\epsilon)N_1$$

and

$$\|\mathscr{V}^{(m)}_{N_1N_2}\|_2=\|(\mathscr{S}^{(m)}_2)^{-1}\bar{\mathscr{V}}^{(m)}_{N_1N_2}\|_2\leq\|(\mathscr{S}^{(m)}_2)^{-1}\|_2\|\bar{\mathscr{V}}^{(m)}_{N_1N_2}\|_2<\epsilon\,,$$

with the last inequality following from Lemma 3.2. □

Thus fast convergence of the Krylov subspace method for solving the preconditioned system (3.1) can be expected if the diffusion coefficients of the FDE are constants. Incidentally, the proof of Theorem 3.2 cannot be extended directly for the case with variable diffusion coefficients, but the proposed preconditioner still works well for variable diffusion coefficients with sufficiently small variations — although maybe not if the diffusion coefficients have large variations.

4. 3D FDE and Level-3 Circulant Preconditioner

We now consider the following 3D FDE problem:

$$\begin{cases}\dfrac{\partial u(x,y,z,t)}{\partial t}=d_+(x,y,z,t)\dfrac{\partial^{\alpha}u(x,y,z,t)}{\partial_+x^{\alpha}}+d_-(x,y,z,t)\dfrac{\partial^{\alpha}u(x,y,z,t)}{\partial_-x^{\alpha}}\\ \qquad\qquad+e_+(x,y,z,t)\dfrac{\partial^{\beta}u(x,y,z,t)}{\partial_+y^{\beta}}+e_-(x,y,z,t)\dfrac{\partial^{\beta}u(x,y,z,t)}{\partial_-y^{\beta}}\\ \qquad\qquad+r_+(x,y,z,t)\dfrac{\partial^{\gamma}u(x,y,z,t)}{\partial_+z^{\gamma}}+r_-(x,y,z,t)\dfrac{\partial^{\gamma}u(x,y,z,t)}{\partial_-z^{\gamma}}+f(x,y,z,t)\,,\\ \qquad(x,y,z)\in\Omega\,,\qquad t\in(0,T]\,,\\ u(x,y,z,t)=0\,,\qquad(x,y,z)\in\partial\Omega\,,\quad t\in(0,T]\,,\\ u(x,y,z,0)=u_0(x,y,z)\,,\qquad(x,y,z)\in\bar{\Omega}\,.\end{cases}\tag{4.1}$$

Using the same finite difference technique to discretise the above 3D FDE, one can write the numerical scheme in the following matrix form:

$$\Big(\mathscr{I}_{N_1N_2N_3}-\mathscr{A}^{(m)}_x-\mathscr{A}^{(m)}_y-\mathscr{A}^{(m)}_z\Big)\mathbf{u}^{(m)}=\mathbf{u}^{(m-1)}+\Delta t\mathbf{f}^{(m)}\,,\tag{4.2}$$

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where

$$\mathcal{A}_x^{(m)} = \nu_1 \mathrm{diag}(\mathbf{d}_+^{(m)})(\mathcal{I}_{N_3} \otimes \mathcal{I}_{N_2} \otimes \mathcal{G}_\alpha) + \nu_1 \mathrm{diag}(\mathbf{d}_-^{(m)})(\mathcal{I}_{N_3} \otimes \mathcal{I}_{N_2} \otimes \mathcal{G}_\alpha^T),$$
$$\mathcal{A}_y^{(m)} = \nu_2 \mathrm{diag}(\mathbf{e}_+^{(m)})(\mathcal{I}_{N_3} \otimes \mathcal{G}_\beta \otimes \mathcal{I}_{N_1}) + \nu_2 \mathrm{diag}(\mathbf{e}_-^{(m)})(\mathcal{I}_{N_3} \otimes \mathcal{G}_\beta^T \otimes \mathcal{I}_{N_1}),$$
$$\mathcal{A}_z^{(m)} = \nu_3 \mathrm{diag}(\mathbf{r}_+^{(m)})(\mathcal{G}_\gamma \otimes \mathcal{I}_{N_2} \otimes \mathcal{I}_{N_1}) + \nu_3 \mathrm{diag}(\mathbf{r}_-^{(m)})(\mathcal{G}_\gamma^T \otimes \mathcal{I}_{N_2} \otimes \mathcal{I}_{N_1}).$$

From the Remark 2.1 in Section 2, the difference scheme (4.2) is uniquely solvable, unconditionally stable and first-order convergent in the infinity norm. The matrix-vector product of the coefficient matrix in linear system (4.2) with any vector can be obtained in $O(N \log N)$ operations [54], and $O(N)$ memory where $N = N_1 N_2 N_3$, so in solving (4.2) using the Krylov subspace method the operation cost per iteration is $O(N \log N)$. In order to accelerate the convergence rate of the Krylov subspace method, the following level-3 circulant preconditioner $\mathcal{S}_3^{(m)}$ is proposed:

$$\begin{aligned}\mathcal{S}_3^{(m)} =& \mathcal{I}_{N_1 N_2 N_3} - \mathcal{I}_{N_3} \otimes \mathcal{I}_{N_2} \otimes \nu_1 \left[\bar{d}_+^{(m)} s(\mathcal{G}_\alpha) + \bar{d}_-^{(m)} s(\mathcal{G}_\alpha^T) \right] \\ & - \mathcal{I}_{N_3} \otimes \nu_2 \left[\bar{e}_+^{(m)} s(\mathcal{G}_\beta) + \bar{e}_-^{(m)} s(\mathcal{G}_\beta^T) \right] \otimes \mathcal{I}_{N_1} \\ & - \nu_3 \left[\bar{r}_+^{(m)} s(\mathcal{G}_\gamma) + \bar{r}_-^{(m)} s(\mathcal{G}_\gamma^T) \right] \otimes \mathcal{I}_{N_2} \otimes \mathcal{I}_{N_1},\end{aligned}$$

where $\bar{d}_\pm^{(m)}$, $\bar{e}_\pm^{(m)}$ and $\bar{r}_\pm^{(m)}$ are the mean values of the vector $\mathbf{d}_\pm^{(m)}$, $\mathbf{e}_\pm^{(m)}$ and $\mathbf{r}_\pm^{(m)}$, respectively. Similarly, one can prove that $\mathcal{S}_3^{(m)}$ is nonsingular.

Lemma 4.1. *For any vector* $\mathbf{v}$*, the matrix-vector product*

$$\left(\mathcal{S}_3^{(m)}\right)^{-1}\mathbf{v} = (\mathcal{F}_{N_3} \otimes \mathcal{F}_{N_2} \otimes \mathcal{F}_{N_1})^* \left(\Lambda_{s_3}^{(m)}\right)^{-1} (\mathcal{F}_{N_3} \otimes \mathcal{F}_{N_2} \otimes \mathcal{F}_{N_1})\mathbf{v}$$

can be computed in $O(N_1 N_2 N_3 \log N_1 N_2 N_3)$ *operations by using the 3D FFT.*

A MATLAB code to compute the product $(\mathcal{F}_{N_3} \otimes \mathcal{F}_{N_2} \otimes \mathcal{F}_{N_1})\mathbf{v}$ for $N_1 = N_2 = N_3 = N$ is:

```
% Computes 3D FFT
z = reshape(v,N,N^2);
z = fft(z); z = z.';
z = reshape(z,N,N^2);
z = fft(z); z = z.';
z = reshape(z,N,N^2);
z = fft(z); z = z.';
z = reshape(z,N^3,1);
```

For the $N_1 N_2 N_3$-by-$N_1 N_2 N_3$ preconditioned matrix $(\mathcal{S}_3^{(m)})^{-1}\mathcal{M}^{(m)}$, we similarly obtain the following theorem as for Theorem 3.2.

Theorem 4.1. *Assuming that all diffusion coefficients in the FDE* (4.1) *are independent of* $\{x, y, z\}$ *and* $\nu_1, \nu_2, \nu_3 \le \nu$*, for any* $\epsilon > 0$ *there exist* N_1'*,* N_2' *and* N_3' *such that for all* $N_1 > N_1'$*,* $N_2 > N_2'$ *and* $N_3 > N_3'$ *we have*

$$(\mathcal{S}_3^{(m)})^{-1}\mathcal{M}^{(m)} = \mathcal{I} + \mathcal{U}^{(m)} + \mathcal{V}^{(m)},$$

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where

$$\text{rank}(\mathscr{U}^{(m)}) = O(N_1N_2 + N_2N_3 + N_1N_3), \quad \textit{and} \quad ||\mathscr{V}^{(m)}||_2 < \epsilon\ .$$

Thus fast convergence of the preconditioned Krylov subspace method can be expected. However, the rank of $\mathscr{U}^{(m)}$ in Theorem 4.1 increases faster than that in Theorem 3.2, so the convergence rate in the 3D case may be slower than in the 2D case.

Remark 4.1. For d-dimensional FDE, the level-d circulant preconditioner $\mathscr{S}_d^{(m)}$ can be defined similarly. It can be shown that $\mathscr{S}_d^{(m)}$ is nonsingular and the matrix-vector product

$$\left(\mathscr{S}_d^{(m)}\right)^{-1}\mathbf{v} = (\mathscr{F}_{N_d} \otimes \mathscr{F}_{N_{d-1}} \otimes \cdots \otimes \mathscr{F}_{N_1})^*\left(\Lambda_{s_d}^{(m)}\right)^{-1}(\mathscr{F}_{N_d} \otimes \mathscr{F}_{N_{d-1}} \otimes \cdots \otimes \mathscr{F}_{N_1})\mathbf{v}$$

can be computed in $O(N \log N)$ operations using the FFT, where $N = N_1N_2 \cdots N_d$. At the same time, the preconditioned matrix can be expressed as a sum of the identity matrix, a matrix with small norm, and a matrix with low rank.

5. Numerical Examples

In this section, we discuss the numerical solution of the FDE problems (2.1) and (4.1) by the implicit finite difference scheme given in Section 2. At each time level, the preconditioned linear system $(\mathscr{S}_d^{(m)})^{-1}\mathscr{M}^{(m)}\mathbf{u}^{(m)} = (\mathscr{S}_d^{(m)})^{-1}(\mathbf{u}^{(m-1)} + \Delta t\mathbf{f}^{(m)})$ of dimension d was solved using the PGMRES method [43] implemented in MATLAB via the built-in function “gmres" without restart. The stopping criterion of the PGMRES method chosen was $\|\mathbf{r}^{(k)}\|_2/\|\mathbf{r}^{(0)}\|_2 < 10^{-7}$, where $\mathbf{r}^{(k)}$ denotes the residual vector of the linear system after k iterations, and the initial guess at each time step was chosen as the zero vector. All numerical experiments were run in MATLAB 7.13 (R2011b) on a Dell workstation Precision T7500 with the configuration: Intel(R) Xeon(R) CPU X5690 3.47GHz and 12 GB RAM.

In the following, errors between numerical and analytic solutions, numbers of iterations required for convergence, and the corresponding CPU time are reported. In the tables, “N" denotes the number of spatial grid points in each direction — i.e. $N_1 = N_2 = N_3 = N$, “M" denotes the number of time steps, “E_∞" denotes the error between the true solution and the approximation under the infinity norm, “CPU(s)" denotes the total CPU time in seconds for solving the FDE problems, and “Iter" denotes the average number of iterations. For comparison, we also report the numerical results from the the GMRES method without any preconditioner (denoted as “GMRES" in all tables), and from the preconditioned GMRES (PGMRES) method with the following Chan-based preconditioner $\mathscr{C}_d^{(m)}$ (denoted as “PGMRES(C)" in all tables):

$$\mathscr{C}_2^{(m)} = \mathscr{I}_{N_1N_2} - \mathscr{I}_{N_2} \otimes \nu_1\left[\bar{d}_+^{(m)}c(\mathscr{G}_\alpha) + \bar{d}_-^{(m)}c(\mathscr{G}_\alpha^T)\right] - \nu_2\left[\bar{e}_+^{(m)}c(\mathscr{G}_\beta) + \bar{e}_-^{(m)}c(\mathscr{G}_\beta^T)\right] \otimes \mathscr{I}_{N_1}\ ,$$

and

$$\begin{aligned}\mathscr{C}_3^{(m)} =& \mathscr{I}_{N_1N_2N_3} - \mathscr{I}_{N_3} \otimes \mathscr{I}_{N_2} \otimes \nu_1\left[\bar{d}_+^{(m)}c(\mathscr{G}_\alpha) + \bar{d}_-^{(m)}c(\mathscr{G}_\alpha^T)\right] \\ & - \mathscr{I}_{N_3} \otimes \nu_2\left[\bar{e}_+^{(m)}c(\mathscr{G}_\beta) + \bar{e}_-^{(m)}c(\mathscr{G}_\beta^T)\right] \otimes \mathscr{I}_{N_1} - \nu_3\left[\bar{s}_+^{(m)}c(\mathscr{G}_\gamma) + \bar{s}_-^{(m)}c(\mathscr{G}_\gamma^T)\right] \otimes \mathscr{I}_{N_2} \otimes \mathscr{I}_{N_1},\end{aligned}$$

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where $c(\cdot)$ denotes the Chan's circulant preconditioner [10] for a Toeplitz matrix. In passing, we note that $\mathscr{C}_2$ has been used recently as the preconditioner [16]. The assumed first columns of the circulant matrices $c(\mathscr{G}_\xi)$ were

$$\frac{1}{N_i}\begin{pmatrix} N_i g_1^{(\xi)} \\ (N_i-1)g_2^{(\xi)} \\ \vdots \\ 2g_{N_i-1}^{(\xi)} \\ g_{N_i}^{(\xi)} + (N_i-1)g_0^{(\xi)} \end{pmatrix}, \quad \text{for } (i,\xi) = (1,\alpha),(2,\beta),(3,\gamma)\,.$$

In Example 5.1, we also report the CPU time for solving the linear system (2.6) using a direct method (left division in MATLAB), denoted as "Direct" in Table 1 and Table 2.

Two numerical examples are reported in the following. The first one is in 2D and the second one is in 3D. The time domain for all examples was $[0,T]$ with $T=1$, and the spatial domain $\Omega=[0,1]^d$. For the time step and space steps, we chose

$$h_1 = h_2 = h_3 = h = \frac{1}{N+1} \quad \text{and} \quad M = N\,,$$

so that $\Delta t = 1/M \approx h$.

Example 5.1. In this example, we test the FDE problem (2.1) with the exact solution

$$u(x,y,t) = e^{-t}x^3(1-x)^3y^3(1-y)^3\,.$$

The source term $f(x,y,t)$ was determined using the above exact solution, with the initial condition $u_0(x,y) = x^3(1-x)^3y^3(1-y)^3$. The following two sets of diffusion coefficients were considered in our tests:

(i) $d_+ = 0.9$, $d_- = 0.6$, $e_+ = 0.7$, $e_- = 0.8$;

(ii) $d_+ = x^\alpha(1-y)e^{-t}$, $d_- = (1-x)^\alpha y e^{-t}$, $e_+ = (1-x)y^\beta e^{-t}$, $e_- = x(1-y)^\beta e^{-t}$,

and the numerical results are reported in Tables 1 and 2, respectively.

Example 5.2. In this example, we consider the 3D FDE (4.1) with the exact solution

$$u(x,y,z,t) = e^{-t}x^3(1-x)^3y^3(1-y)^3z^3(1-z)^3\,.$$

The source term $f(x,y,z,t)$ was determined from the above exact solution, with the initial condition $u_0(x,y,z) = x^3(1-x)^3y^3(1-y)^3z^3(1-z)^3$. Table 3 shows the numerical result with $d_\pm = e_\pm = s_\pm = 1$.

From Tables 1 and 2, one can see there is first-order convergence of the difference scheme in the infinity norm. On efficiency, the CPU time of the GMRES method with no preconditioner is much less than that of the direct method, due to the fast matrix-vector product algorithm and the storage reduction suggested in Ref. [57]. However, the coefficient matrix is ill-conditioned such that the number of iteration of the GMRES method

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Table 1: Numerical results for Example 5.1 with $d_+ = 0.9, d_- = 0.6, e_+ = 0.7, e_- = 0.8$.

			Direct	GMRES		PGMRES(C)		PGMRES(S)	
N	E_∞	Rate	CPU(s)	Iter	CPU(s)	Iter	CPU(s)	Iter	CPU(s)
$\alpha = 1.1, \beta = 1.2$									
2^4	3.2253e-05	-	0.06	21.0	0.30	9.0	0.22	8.9	0.22
2^5	2.0450e-05	0.6573	1.39	23.0	0.72	9.0	0.37	8.8	0.38
2^6	1.1689e-05	0.8069	61.70	23.0	3.81	8.0	1.65	8.0	1.67
2^7	6.2918e-06	0.8936	4024.60	23.0	20.75	7.9	8.82	8.0	9.00
2^8	3.2705e-06	0.9440	-	22.0	204.14	7.0	79.98	7.0	80.68
2^9	1.6682e-06	0.9712	-	-	-	6.8	711.24	6.9	719.45
$\alpha = 1.4, \beta = 1.5$									
2^4	7.5324e-06	-	0.05	29.9	0.40	11.0	0.24	10.9	0.24
2^5	4.3232e-06	0.8010	1.46	39.0	1.35	12.0	0.47	11.0	0.45
2^6	2.3134e-06	0.9021	62.49	50.9	10.65	12.0	2.31	11.0	2.12
2^7	1.1983e-06	0.9490	4024.84	59.0	73.91	11.8	12.14	11.0	11.31
2^8	6.0970e-07	0.9748	-	68.0	970.24	10.0	104.40	10.0	104.40
2^9	3.0751e-07	0.9875	-	-	-	10.0	977.89	9.0	895.47
$\alpha = 1.8, \beta = 1.9$									
2^4	4.9754e-07	-	0.05	39.0	0.53	14.0	0.27	12.0	0.25
2^5	1.5329e-07	1.6985	1.43	67.0	2.85	17.0	0.65	13.0	0.51
2^6	1.0216e-07	0.5855	62.47	105.0	33.44	20.0	3.76	13.0	2.48
2^7	6.2547e-08	0.7078	4028.37	165.0	416.33	25.0	25.86	14.0	13.89
2^8	3.4396e-08	0.8627	-	229.0	8032.65	27.0	282.72	15.0	149.95
2^9	1.8003e-08	0.9340	-	-	-	28.0	2960.59	15.0	1436.66
$\alpha = 1.2, \beta = 1.8$									
2^4	5.1099e-06	-	0.05	40.0	0.54	15.0	0.28	13.0	0.26
2^5	3.0157e-06	0.7608	1.48	58.0	2.30	17.0	0.64	14.9	0.58
2^6	1.6434e-06	0.8758	62.82	80.0	21.56	17.9	3.38	16.0	3.01
2^7	8.5759e-07	0.9383	4029.68	109.0	202.14	18.0	17.80	15.8	15.53
2^8	4.3811e-07	0.9690	-	138.0	3208.21	18.0	179.10	14.0	139.98
2^9	2.2142e-07	0.9845	-	-	-	17.0	1636.53	14.0	1333.70

is large. After invoking the level-2 circulant preconditioners $\mathscr{S}_2^{(m)}$ and $\mathscr{C}_2^{(m)}$, the number of iterations and the CPU time of the PGMRES method are reduced significantly, and the performance on using the preconditioner $\mathscr{S}_2^{(m)}$ is best.

From Table 3, the first-order convergence rate of the difference scheme in the infinity norm can also be seen. Meanwhile, in contrast with $\mathscr{C}_3^{(m)}$, the preconditioner $\mathscr{S}_3^{(m)}$ is still powerful in speeding up the convergence, demonstrating that fast convergence of the PGMRES method for d-dimensional FDE can be expected.

6. Conclusions

An implicit finite difference scheme for solving two-sided FDE with nonnegative variable diffusion coefficients has been studied. The scheme was proven to be unconditionally stable and first-order convergent in the infinity norm. Further, the discretised linear system at each time level was solved using the PGMRES method with the proposed multilevel cir-

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Table 2: Numerical results for Example 5.1 with $d_+ = x^\alpha(1-y)e^{-t}$, $d_- = (1-x)^\alpha y e^{-t}$, $e_+ = (1-x)y^\beta e^{-t}$, $e_- = x(1-y)^\beta e^{-t}$.

			Direct	GMRES		PGMRES(C)		PGMRES(S)	
N	E_∞	Rate	CPU(s)	Iter	CPU(s)	Iter	CPU(s)	Iter	CPU(s)
$\alpha = 1.1, \beta = 1.2$									
2^4	1.6518e-05	-	0.07	13.8	0.22	11.6	0.26	11.6	0.25
2^5	1.1104e-05	0.5729	2.07	17.0	0.55	11.4	0.46	11.3	0.47
2^6	6.5844e-06	0.7540	83.59	18.4	3.08	10.2	2.06	10.0	2.02
2^7	3.6203e-06	0.8630	4662.27	18.4	17.27	9.1	10.44	8.9	10.28
2^8	1.9047e-06	0.9265	-	17.9	170.96	8.4	93.62	8.1	91.96
2^9	9.7806e-07	0.9616	-	-	-	7.6	818.86	7.4	796.10
$\alpha = 1.4, \beta = 1.5$									
2^4	4.3073e-06	-	0.08	19.8	0.28	13.1	0.27	13.5	0.27
2^5	2.1993e-06	0.9698	2.07	27.8	0.93	14.3	0.56	13.9	0.55
2^6	1.1162e-06	0.9785	83.22	36.9	7.02	14.6	2.80	14.1	2.72
2^7	5.6261e-07	0.9883	4663.75	46.6	55.12	14.0	14.83	13.5	14.28
2^8	2.8248e-07	0.9940	-	56.6	762.82	13.1	136.22	12.6	131.99
2^9	1.4155e-07	0.9969	-	-	-	12.4	1240.86	11.9	1195.70
$\alpha = 1.8, \beta = 1.9$									
2^4	3.6501e-06	-	0.08	31.1	0.43	17.8	0.33	16.2	0.30
2^5	1.6325e-06	1.1609	2.00	49.7	1.91	20.2	0.78	18.1	0.70
2^6	7.6862e-07	1.0867	82.98	76.8	20.35	21.0	4.04	19.1	3.67
2^7	3.7407e-07	1.0390	4670.34	112.4	222.37	21.1	22.28	19.2	19.79
2^8	1.8464e-07	1.0186	-	156.4	4136.50	20.7	214.60	18.5	191.01
2^9	9.1737e-08	1.0091	-	-	-	19.6	2002.82	17.7	1789.35
$\alpha = 1.2, \beta = 1.8$									
2^4	5.2478e-06	-	0.08	25.8	0.36	16.1	0.30	15.8	0.30
2^5	2.8399e-06	0.8859	2.04	39.0	1.39	17.8	0.69	17.2	0.67
2^6	1.4820e-06	0.9383	83.19	55.1	12.38	17.9	3.43	17.2	3.31
2^7	7.5949e-07	0.9644	4670.58	75.6	115.20	17.3	18.15	16.6	17.29
2^8	3.8447e-07	0.9822	-	100.4	1918.81	16.4	168.92	15.6	160.98
2^9	1.9343e-07	0.9911	-	-	-	15.1	1512.81	14.2	1421.64

culant preconditioner $\mathscr{S}_d^{(m)}$. The preconditioner is nonsingular, and can be constructed and applied easily (just a few lines in MATLAB). In general, the matrix-vector product $(\mathscr{S}_d^{(m)})^{-1}\mathbf{v}$ (for any real vector $\mathbf{v}$) can be computed in $O(N \log N)$ operations using the FFT such that the operation cost for each iteration is $O(N \log N)$, where $N = N_1 N_2 \cdots N_d$. Moreover, if the diffusion coefficients are constants, the preconditioned matrix can be written as a sum of the identity matrix, a matrix with small norm and a matrix with low rank, so that fast convergence of the PGMRES method can be expected. Numerical tests revealed the effectiveness of the preconditioner.

Moreover, due to the similar structure of the coefficient matrix, the proposed preconditioner can be applied to implicit finite difference schemes with high-order fractional derivatives approximations [12, 48, 52, 53, 58, 60], and to solve FDE with a nonlinear reaction term [24]. However, the proposed preconditioner may not good enough if the variation of the diffusion coefficients is large, which is an issue for further investigation.

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Table 3: Numerical results for Example 5.2 with all diffusion coefficients equal to 1.

			GMRES		PGMRES(C)		PGMRES(S)	
N	E_∞	Rate	Iter	CPU(s)	Iter	CPU(s)	Iter	CPU(s)
	$\alpha = 1.1, \beta = 1.2, \gamma = 1.3$							
2^4	3.8419e-07	-	25.0	0.99	11.0	0.56	10.0	0.51
2^5	2.4335e-07	0.6588	32.0	13.83	11.0	5.33	10.0	4.60
2^6	1.3877e-07	0.8104	36.0	374.59	10.0	97.87	9.0	89.92
2^7	7.4445e-08	0.8984	38.0	7536.08	9.9	1709.89	9.0	1568.02
	$\alpha = 1.4, \beta = 1.5, \gamma = 1.6$							
2^4	8.9517e-08	-	31.8	1.29	13.0	0.65	11.0	0.59
2^5	5.3309e-08	0.7478	49.0	25.98	15.0	7.33	12.0	5.42
2^6	2.8952e-08	0.8807	69.5	1033.85	17.0	161.35	12.0	114.28
2^7	1.5068e-08	0.9422	91.0	31737.99	17.0	2987.701	12.0	2070.86
	$\alpha = 1.7, \beta = 1.8, \gamma = 1.9$							
2^4	6.6980e-09	-	38.9	1.81	15.0	0.72	11.0	0.58
2^5	4.5709e-09	0.5513	69.0	46.64	20.0	8.53	14.0	5.97
2^6	3.3264e-09	0.4585	118.0	2585.55	26.0	267.13	14.0	132.02
2^7	1.9347e-09	0.7819	190.0	120791.15	32.0	6620.07	16.0	2799.63
	$\alpha = 1.2, \beta = 1.5, \gamma = 1.8$							
2^4	8.0314e-08	-	39.0	1.74	16.0	0.77	11.1	0.56
2^5	4.8481e-08	0.7282	63.0	39.99	19.0	8.18	14.0	5.91
2^6	2.6493e-08	0.8718	93.0	1691.22	22.0	217.34	15.0	142.79
2^7	1.3829e-08	0.9379	129.0	59328.07	24.0	4519.45	15.0	2618.08

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