

## WSLD operators: A class of fourth order difference approximations for space Riemann-Liouville derivative

MINGHUA CHEN AND WEIHUA DENG<sup>†</sup>

*School of Mathematics and Statistics, Lanzhou University, Lanzhou 730000, P. R. China*

[Received on 18 July 2018]

Because of the nonlocal properties of fractional operators, higher order schemes play more important role in discretizing fractional derivatives than classical ones. The striking feature is that higher order schemes of fractional derivatives can keep the same computation cost with first-order schemes but greatly improve the accuracy. Nowadays, there are already two types of second order discretization schemes for space fractional derivatives: the first type is given and discussed in [Sousa & Li, arXiv:1109.2345; Chen & Deng, arXiv:1304.3788; Chen et al., Appl. Numer. Math., 70, 22-41]; and the second type is a class of schemes presented in [Tian et al., arXiv:1201.5949]. The core object of this paper is to derive a class of fourth order approximations, called the weighted and shifted Lubich difference (WSLD) operators, for space fractional derivatives. Then we use the derived schemes to solve the space fractional diffusion equation with variable coefficients in one-dimensional and two-dimensional cases. And the unconditional stability and the convergence with the global truncation error  $\mathcal{O}(\tau^2 + h^4)$  are theoretically proved and numerically verified.

*Keywords:* Fractional diffusion equation; Weighted and shifted Lubich difference operators; Numerical stability; Convergence

### 1. Introduction

In recent decades, fractional operators have been playing more and more important roles [Diethelm (2010)], e.g., in mechanics (theory of viscoelasticity and viscoplasticity), (bio-)chemistry (modelling of polymers and proteins), electrical engineering (transmission of ultrasound waves), medicine (modelling of human tissue under mechanical loads), etc. Efficiently solving the fractional partial differential equations (PDEs) naturally becomes an urgent topic. Because of the nonlocal properties of fractional operators, obtaining the analytical solutions of the fractional PDEs is more challenge or sometimes even impossible; or the obtained analytical solutions are less valuable (expressed by transcendental functions or infinite series). Luckily, some important progress has been made for numerically solving the fractional PDEs by finite difference methods, e.g., see [Meerschaert & Tadjeran (2004); Sousa & Li (2011); Sun & Wu (2006); Tian *et al.* (2012); Yuste (2006); Zhuang *et al.* (2009)].

In solving space fractional PDEs, high order finite difference schemes display more striking benefits because most of the time they can use the same computational cost with first order scheme but greatly improve the accuracy. For example, comparing with first order difference scheme which may have the matrix algebraic equation  $(I - A)u^{n+1} = u^n + b^{n+1}$ , the high order scheme has the matrix algebraic equation  $(I - \tilde{A})u^{n+1} = (I + \tilde{B})u^n + \tilde{b}^{n+1/2}$ . The three matrices  $A$ ,  $\tilde{A}$  and  $\tilde{B}$  are all Toeplitz-like and have completely same structure, and the computational count for matrix vector multiplication is

<sup>†</sup>Corresponding author. Email: dengwh@lzu.edu.cn

$\mathcal{O}(N \log N)$ , then the computational costs for solving the two matrix algebraic equations are almost the same [Chen *et al.* (2012)].

Nowadays, we notice that there exist two types of second order discretization schemes for space fractional derivatives. The idea of the first type is to combine the centered difference scheme of second classical derivative with piecewise linear polynomial approximation of the fractional integral. Sousa & Li (2011) firstly use the idea to obtain the second order approximation in infinite domain. The paper [Chen & Deng (2011)] detailedly analyzes the effectiveness of the approximation in finite domain. And this discretization is also effectively used to solve the time-space Caputo-Riesz fractional diffusion equation [Chen *et al.* (2013)]. The second type of second order approximation is in fact a class of second order discretization, which are obtained by assembling the Grünwald difference operators with different weights and shifts. This class of approximations are detailedly discussed and successfully applied to solve space fractional diffusion equations in [Tian *et al.* (2012)], and called WSGD operators there. Both of the two types of the operators have completely same structure, and the real parts of the eigenvalues of the matrixes are less than 0, see [Deng & Chen (2013); Tian *et al.* (2012)]. So they can be efficiently used to solve space fractional PDEs.

Based on Lubich's operator [Lubich (1986)], this paper derives a class of fourth order approximations for space fractional derivatives, termed the weighted and shifted Lubich difference operators (WSLD operators). Using the fractional linear multistep methods, Lubich (1986) obtains the  $L$ -th order ( $L \leq 6$ ) approximations of the  $\alpha$ -th derivative ( $\alpha > 0$ ) or integral ( $\alpha < 0$ ) by the corresponding coefficients of the generating functions  $\delta^\alpha(\zeta)$ , where

$$\delta^\alpha(\zeta) = \left( \sum_{i=1}^L \frac{1}{i} (1-\zeta)^i \right)^\alpha. \quad (1.1)$$

For  $\alpha = 1$ , the scheme reduces to the classical  $(L+1)$ -point backward difference formula [Henrici (1962)]. For  $L = 1$ , the scheme (1.1) corresponds to the standard Grünwald discretization of  $\alpha$ -th derivative with first order accuracy; unfortunately, for the time dependent equations the difference scheme is unstable. But Meerschaert & Tadjeran (2004) successfully circumvent this difficulties by the so-called shifted Grünwald formulae. Taking  $L = 2$ , Cuesta *et al.* (2006) discuss the convolution quadrature time discretization of fractional diffusion-wave equations; when applying the discretization scheme to space fractional operator with  $\alpha \in (1, 2)$  for time dependent problem, the obtained scheme is also unstable, since the eigenvalues of the matrix corresponding to the discretized operator are greater than one. If using the shifted Lubich's formula, it reduces to the first order accuracy (detailed description is given in Section 2). This paper weights and shifts Lubich's operator to obtain a class of fourth order discretization schemes, which are effective for time dependent problem. Then we use the fourth order schemes to solve the following two-dimensional fractional diffusion equation with variable coefficients,

$$\begin{cases} \frac{\partial u(x,y,t)}{\partial t} = d_+(x,y)_{x_L} D_x^\alpha u(x,y,t) + d_-(x,y)_x D_{x_R}^\alpha u(x,y,t) \\ \quad + e_+(x,y)_{y_L} D_y^\beta u(x,y,t) + e_-(x,y)_y D_{y_R}^\beta u(x,y,t) + f(x,y,t), \\ u(x,y,0) = u_0(x,y), \quad \text{for } (x,y) \in \Omega, \\ u(x,y,t) = 0, \quad \text{for } (x,y,t) \in \partial\Omega \times (0,T], \end{cases} \quad (1.2)$$

in the domain  $\Omega = (x_L, x_R) \times (y_L, y_R)$ ,  $0 < t \leq T$ , where the orders of the fractional derivatives are  $1 < \alpha, \beta < 2$  and  $f(x,y,t)$  is a source term, and all the variable coefficients are nonnegative. The left

and right Riemann-Liouville fractional derivatives of the function  $u(x)$  on  $[x_L, x_R]$ ,  $-\infty \leq x_L < x_R \leq \infty$  are, respectively, defined by [Podlubny (1999); Samko *et al.* (1993)]

$${}_{x_L}D_x^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_{x_L}^x (x-\xi)^{1-\alpha} u(\xi) d\xi, \quad (1.3)$$

and

$${}_{x_R}D_x^\alpha u(x) = \frac{1}{\Gamma(2-\alpha)} \frac{\partial^2}{\partial x^2} \int_x^{x_R} (\xi-x)^{1-\alpha} u(\xi) d\xi. \quad (1.4)$$

The outline of this paper is as follows. In Section 2, we derive a class of fourth order approximations for space fractional Riemann-Liouville derivatives, being effective in solving space fractional PDEs. In Section 3, the full discretization schemes of one-dimensional case of (1.2) and (1.2) itself are presented. Section 4 does the detailed theoretical analyses for the stability and convergence of the given schemes. To show the effectiveness of the algorithm, we perform the numerical experiments to verify the theoretical results in Section 5. Finally, we conclude the paper with some remarks in the last section.

## 2. Derivation of a class of fourth order discretizations for space fractional operators

In the following, we derive a class of fourth order approximations for Riemann-Liouville fractional derivatives, and prove that they are effective in solving space fractional PDE, i.e., all the eigenvalues of the matrixes corresponding to the discretized operators have negative real parts.

### 2.1 Derivation of the discretization scheme

Taking  $L = 2$ , for all  $|\zeta| \leq 1$ , Eq. (1.1) can be recast as

$$\begin{aligned} \left(\frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2\right)^\alpha &= \left(\frac{3}{2}\right)^\alpha (1-\zeta)^\alpha \left(1 - \frac{1}{3}\zeta\right)^\alpha \\ &= \left(\frac{3}{2}\right)^\alpha \sum_{n=0}^{\infty} (-1)^n \binom{\alpha}{n} \zeta^n \cdot \sum_{m=0}^{\infty} \left(-\frac{1}{3}\right)^m \binom{\alpha}{m} \zeta^m \\ &= \left(\frac{3}{2}\right)^\alpha \sum_{n=0}^{\infty} \left[ \sum_{m=0}^{\infty} (-1)^n \binom{\alpha}{n} \cdot \left(-\frac{1}{3}\right)^m \binom{\alpha}{m} \right] \zeta^{m+n} \\ &= \sum_{k=0}^{\infty} q_k^\alpha \zeta^k, \end{aligned} \quad (2.1)$$

with  $k = m + n$ , and

$$q_k^\alpha = (-1)^k \left(\frac{3}{2}\right)^\alpha \sum_{m=0}^k 3^{-m} \binom{\alpha}{k-m} \binom{\alpha}{m} = \left(\frac{3}{2}\right)^\alpha \sum_{m=0}^k 3^{-m} g_m^\alpha g_{k-m}^\alpha, \quad (2.2)$$

where  $g_k^\alpha = (-1)^k \binom{\alpha}{k}$  are the coefficients of the power series of the generating function  $(1-\zeta)^\alpha$ , and they can be calculated by the following recursively formula

$$g_0^\alpha = 1, \quad g_k^\alpha = \left(1 - \frac{\alpha+1}{k}\right) g_{k-1}^\alpha, \quad k \geq 1. \quad (2.3)$$

If  $\alpha < 0$ ,  $\{q_k^\alpha\}_{k=0}^\infty$  correspond to the coefficients of the 2nd order convolution quadrature for the approximation of fractional integral operator [see, Cuesta *et al.* (2006)].

LEMMA 2.1 The coefficients in (2.2) with  $\alpha \in (1, 2)$  satisfy the following properties

$$\begin{aligned} q_0^\alpha &= \left(\frac{3}{2}\right)^\alpha > 0; & q_1^\alpha &= -\left(\frac{3}{2}\right)^\alpha \frac{4\alpha}{3} < 0; \\ q_2^\alpha &= \left(\frac{3}{2}\right)^\alpha \frac{\alpha(8\alpha-5)}{9} > 0; & q_3^\alpha &= \left(\frac{3}{2}\right)^\alpha \frac{4\alpha(\alpha-1)(7-8\alpha)}{81} < 0; \\ q_4^\alpha &= \left(\frac{3}{2}\right)^\alpha \frac{\alpha(\alpha-1)(64\alpha^2-176\alpha+123)}{486} > 0; \\ q_5^\alpha &= \left(\frac{3}{2}\right)^\alpha \frac{2\alpha(\alpha-1)(2-\alpha)(64\alpha^2-208\alpha+183)}{3645} > 0; & \sum_{k=0}^\infty q_k^\alpha &= 0. \end{aligned}$$

*Proof.* Taking  $\zeta = 1$ , it is easy to check that

$$\sum_{k=0}^\infty q_k^\alpha = \sum_{k=0}^\infty q_k^\alpha \zeta^k = \left(\frac{3}{2} - 2\zeta + \frac{1}{2}\zeta^2\right)^\alpha = 0.$$

□

We first introduce two lemmas, which will be used to prove that the several classes of derived discretization schemes are 2nd, 3rd, and 4th order convergent, respectively.

LEMMA 2.2 (Ervin & Roop (2006)) Let  $\alpha > 0$ ,  $u \in C_0^\infty(\Omega)$ ,  $\Omega \subset \mathbb{R}$ , then

$$\mathcal{F}(-\infty D_x^\alpha u(x)) = (-i\omega)^\alpha \widehat{u}(\omega) \quad \text{and} \quad \mathcal{F}({}_x D_\infty^\alpha u(x)) = (i\omega)^\alpha \widehat{u}(\omega),$$

where  $\mathcal{F}$  denotes the Fourier transform operator and  $\widehat{u}(\omega) = \mathcal{F}(u)$ , i.e.,

$$\widehat{u}(\omega) = \int_{\mathbb{R}} e^{i\omega x} u(x) dx.$$

LEMMA 2.3 Let  $u$ ,  $-\infty D_x^{\alpha+1} u(x)$  (or  $-\infty D_x^{\alpha+2} u(x)$ ) with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$  when  $p \neq 0$  (or  $p = 0$ ); and denote that

$${}_L A_p^\alpha u(x) = \frac{1}{h^\alpha} \sum_{k=0}^\infty q_k^\alpha u(x - (k-p)h), \quad (2.4)$$

where  $q_k^\alpha$  is defined by (2.2) and  $p$  an integer. Then

$$-\infty D_x^\alpha u(x) = {}_L A_p^\alpha u(x) + \mathcal{O}(h), \quad p \neq 0,$$

and

$$-\infty D_x^\alpha u(x) = {}_L A_p^\alpha u(x) + \mathcal{O}(h^2), \quad p = 0.$$

*Proof.* From (2.2) and  $k = m + n$ , we obtain

$$\begin{aligned}
\mathcal{F}(L A_p^\alpha u)(\omega) &= h^{-\alpha} \sum_{k=0}^{\infty} q_k^\alpha \mathcal{F}(u(x - (k-p)h))(\omega) \\
&= h^{-\alpha} e^{-i\omega p h} \sum_{k=0}^{\infty} q_k^\alpha (e^{i\omega h})^k \widehat{u}(\omega) \\
&= h^{-\alpha} e^{-i\omega p h} \left(\frac{3}{2}\right)^\alpha \sum_{n=0}^{\infty} (-1)^n \binom{\alpha}{n} e^{i\omega n h} \cdot \sum_{m=0}^{\infty} \left(-\frac{1}{3}\right)^m \binom{\alpha}{m} e^{i\omega m h} \widehat{u}(\omega) \\
&= (-i\omega)^\alpha \left[ e^{-i\omega p h} \left(\frac{1 - e^{i\omega h}}{-i\omega h}\right)^\alpha \right] \left(1 + \frac{1}{2}(1 - e^{i\omega h})\right)^\alpha \widehat{u}(\omega) \\
&= (-i\omega)^\alpha e^{pz} \left(\frac{1 - e^{-z}}{z}\right)^\alpha \left(1 + \frac{1}{2}(1 - e^{-z})\right)^\alpha \widehat{u}(\omega),
\end{aligned}$$

with  $z = -i\omega h$ . It is easy to check that

$$\begin{aligned}
e^{pz} \left(\frac{1 - e^{-z}}{z}\right)^\alpha &= \left[1 + \left(p - \frac{\alpha}{2}\right)z + \left(\frac{1}{2}p^2 - \frac{\alpha}{2}p + \frac{3\alpha^2 + \alpha}{24}\right)z^2\right. \\
&\quad \left.+ \left(\frac{1}{6}p^3 - \frac{\alpha}{4}p^2 + \frac{3\alpha^2 + \alpha}{24}p - \frac{\alpha^3 + \alpha^2}{48}\right)z^3 + \mathcal{O}(z^4)\right],
\end{aligned}$$

and

$$\left(1 + \frac{1}{2}(1 - e^{-z})\right)^\alpha = \left[1 + \frac{\alpha}{2}z + \frac{\alpha(\alpha - 3)}{8}z^2 + \frac{\alpha(\alpha^2 - 9\alpha + 12)}{48}z^3 + \mathcal{O}(z^4)\right],$$

then we have

$$e^{pz} \left(\frac{1 - e^{-z}}{z}\right)^\alpha \left(1 + \frac{1}{2}(1 - e^{-z})\right)^\alpha = 1 + pz + \frac{3p^2 - 2\alpha}{6}z^2 + \frac{2p^3 + \alpha(3 - 4p)}{12}z^3 + \mathcal{O}(z^4). \quad (2.5)$$

Therefore, from Lemma 2.1, we get

$$\mathcal{F}(L A_p^\alpha u)(\omega) = \mathcal{F}({}_{-\infty}D_x^\alpha u(x)) + \widehat{\phi}(\omega),$$

where  $\widehat{\phi}(\omega) = (-i\omega)^\alpha \left(pz + \frac{3p^2 - 2\alpha}{6}z^2 + \frac{2p^3 + \alpha(3 - 4p)}{12}z^3 + \mathcal{O}(z^4)\right) \widehat{u}(\omega)$ . Then there exists

$$\begin{aligned}
|\widehat{\phi}(\omega)| &\leq \widetilde{c} |i\omega|^{\alpha+1} |\widehat{u}(\omega)| \cdot h, \quad p \neq 0, \\
|\widehat{\phi}(\omega)| &\leq c |i\omega|^{\alpha+2} |\widehat{u}(\omega)| \cdot h^2, \quad p = 0.
\end{aligned}$$

Hence

$$|{}_{-\infty}D_x^\alpha u(x) - L A_p^\alpha u(x)| = |\phi(x)| \leq \frac{1}{2\pi} \int_{\mathbb{R}} |\widehat{\phi}(\omega)| dx = \begin{cases} \mathcal{O}(h), & p \neq 0, \\ \mathcal{O}(h^2), & p = 0. \end{cases}$$

□

In the following, we present the approximation operators for Riemann-Liouville derivative and prove that they have 2nd, 3rd, and 4th order truncation errors.

**THEOREM 2.1** (Second order approximations for left Riemann-Liouville derivative) Let  $u, {}_{-\infty}D_x^{\alpha+2}u(x)$  with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$ . Denote that

$${}_2L A_{p,q}^\alpha u(x) = w_p {}_L A_p^\alpha u(x) + w_q {}_L A_q^\alpha u(x), \quad (2.6)$$

where  ${}_L A_p^\alpha, {}_L A_q^\alpha$  are defined by (2.4),  $w_p = \frac{q}{q-p}, w_q = \frac{p}{p-q}, p \neq q$ , and  $p, q$  are integers. Then

$${}_{-\infty}D_x^\alpha u(x) = {}_2L A_{p,q}^\alpha u(x) + \mathcal{O}(h^2).$$

*Proof.* From the proof of Lemma 2.3, we have

$$\mathcal{F}({}_L A_p^\alpha u)(\omega) = (-i\omega)^\alpha \left[ 1 + pz + \frac{3p^2 - 2\alpha}{6} z^2 + \frac{2p^3 + \alpha(3-4p)}{12} z^3 + \mathcal{O}(z^4) \right] \widehat{u}(\omega)$$

and

$$\mathcal{F}({}_L A_q^\alpha u)(\omega) = (-i\omega)^\alpha \left[ 1 + qz + \frac{3q^2 - 2\alpha}{6} z^2 + \frac{2q^3 + \alpha(3-4q)}{12} z^3 + \mathcal{O}(z^4) \right] \widehat{u}(\omega).$$

Then there exists

$$\mathcal{F}({}_2L A_{p,q}^\alpha u)(\omega) = (-i\omega)^\alpha \left[ 1 - \frac{3pq + 2\alpha}{6} z^2 - \frac{2pq(p+q) - 3\alpha}{12} z^3 + \mathcal{O}(z^4) \right] \widehat{u}(\omega),$$

and by the similar way to the proof of Lemma 2.3 we get

$${}_{-\infty}D_x^\alpha u(x) = {}_2L A_{p,q}^\alpha u(x) + \mathcal{O}(h^2). \quad \square$$

**THEOREM 2.2** (Third order approximations for left Riemann-Liouville derivative) Let  $u, {}_{-\infty}D_x^{\alpha+3}u(x)$  with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$ . Denote that

$${}_3L A_{p,q,r,s}^\alpha u(x) = w_{p,q} {}_2L A_{p,q}^\alpha u(x) + w_{r,s} {}_2L A_{r,s}^\alpha u(x), \quad (2.7)$$

where  ${}_2L A_{p,q}^\alpha$  and  ${}_2L A_{r,s}^\alpha$  are defined by (2.6),  $w_{p,q} = \frac{3rs+2\alpha}{3(rs-pq)}, w_{r,s} = \frac{3pq+2\alpha}{3(pq-rs)}, rs \neq pq$ , and  $p, q, r, s$  are integers. Then

$${}_{-\infty}D_x^\alpha u(x) = {}_3L A_{p,q,r,s}^\alpha u(x) + \mathcal{O}(h^3).$$

*Proof.* By the proof of Theorem 2.1, we have

$$\mathcal{F}({}_2L A_{p,q}^\alpha u)(\omega) = (-i\omega)^\alpha \left[ 1 - \frac{3pq + 2\alpha}{6} z^2 - \frac{2pq(p+q) - 3\alpha}{12} z^3 + \mathcal{O}(z^4) \right] \widehat{u}(\omega)$$

and

$$\mathcal{F}({}_2L A_{r,s}^\alpha u)(\omega) = (-i\omega)^\alpha \left[ 1 - \frac{3rs + 2\alpha}{6} z^2 - \frac{2rs(r+s) - 3\alpha}{12} z^3 + \mathcal{O}(z^4) \right] \widehat{u}(\omega).$$

Then there exists

$$\begin{aligned} & \mathcal{F}({}_3L A_{p,q,r,s}^\alpha u)(\omega) \\ &= (-i\omega)^\alpha \left[ 1 + \frac{6pqrs(r+s-p-q) + 4\alpha[rs(r+s) - pq(p+q)] + 9\alpha(rs-pq)}{36(rs-pq)} z^3 + \mathcal{O}(z^4) \right] \widehat{u}(\omega), \end{aligned}$$

and by the similar way to the proof of Lemma 2.3 we get

$$-_{\infty}D_x^\alpha u(x) = {}_3LA_{p,q,r,s}^\alpha u(x) + \mathcal{O}(h^3).$$

□

**THEOREM 2.3** (Fourth order approximations for left Riemann-Liouville derivative) Let  $u, -_{\infty}D_x^{\alpha+4}u(x)$  with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$ . Denote that

$${}_4LA_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) = w_{p,q,r,s} {}_3LA_{p,q,r,s}^\alpha u(x) + w_{\bar{p},\bar{q},\bar{r},\bar{s}} {}_3LA_{\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x), \quad (2.8)$$

where  ${}_3LA_{p,q,r,s}^\alpha$  and  ${}_3LA_{\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  are defined by (2.7); and

$$w_{p,q,r,s} = \frac{a_{p,q,r,s} \bar{b}_{\bar{p},\bar{q},\bar{r},\bar{s}}}{a_{p,q,r,s} \bar{b}_{\bar{p},\bar{q},\bar{r},\bar{s}} - \bar{a}_{\bar{p},\bar{q},\bar{r},\bar{s}} b_{p,q,r,s}}; \quad (2.9)$$

$$w_{\bar{p},\bar{q},\bar{r},\bar{s}} = \frac{\bar{a}_{\bar{p},\bar{q},\bar{r},\bar{s}} b_{p,q,r,s}}{\bar{a}_{\bar{p},\bar{q},\bar{r},\bar{s}} b_{p,q,r,s} - a_{p,q,r,s} \bar{b}_{\bar{p},\bar{q},\bar{r},\bar{s}}}; \quad (2.10)$$

with

$$a_{p,q,r,s} = rs - pq; \quad b_{p,q,r,s} = 6pqrs(r+s-p-q) + 4\alpha[rs(r+s) - pq(p+q)] + 9\alpha(rs - pq);$$

$$\bar{a}_{\bar{p},\bar{q},\bar{r},\bar{s}} = \bar{r}\bar{s} - \bar{p}\bar{q}; \quad \bar{b}_{\bar{p},\bar{q},\bar{r},\bar{s}} = 6\bar{p}\bar{q}\bar{r}\bar{s}(\bar{r} + \bar{s} - \bar{p} - \bar{q}) + 4\alpha[\bar{r}\bar{s}(\bar{r} + \bar{s}) - \bar{p}\bar{q}(\bar{p} + \bar{q})] + 9\alpha(\bar{r}\bar{s} - \bar{p}\bar{q});$$

and  $a_{p,q,r,s} \bar{b}_{\bar{p},\bar{q},\bar{r},\bar{s}} \neq \bar{a}_{\bar{p},\bar{q},\bar{r},\bar{s}} b_{p,q,r,s}$ ;  $p, q, r, s; \bar{p}, \bar{q}, \bar{r}, \bar{s}$  are integers. Then

$$-_{\infty}D_x^\alpha u(x) = {}_4LA_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) + \mathcal{O}(h^4).$$

*Proof.* According to the proof of Theorem 2.2, we have

$$\begin{aligned} & \mathcal{F}({}_3LA_{p,q,r,s}^\alpha u)(\omega) \\ &= (-i\omega)^\alpha \left[ 1 + \frac{6pqrs(r+s-p-q) + 4\alpha[rs(r+s) - pq(p+q)] + 9\alpha(rs - pq)}{36(rs - pq)} z^3 + \mathcal{O}(z^4) \right] \hat{u}(\omega) \end{aligned}$$

and

$$\begin{aligned} & \mathcal{F}({}_3LA_{\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u)(\omega) \\ &= (-i\omega)^\alpha \left[ 1 + \frac{6\bar{p}\bar{q}\bar{r}\bar{s}(\bar{r} + \bar{s} - \bar{p} - \bar{q}) + 4\alpha[\bar{r}\bar{s}(\bar{r} + \bar{s}) - \bar{p}\bar{q}(\bar{p} + \bar{q})] + 9\alpha(\bar{r}\bar{s} - \bar{p}\bar{q})}{36(\bar{r}\bar{s} - \bar{p}\bar{q})} z^3 + \mathcal{O}(z^4) \right] \hat{u}(\omega). \end{aligned}$$

Then there exists

$$\mathcal{F}({}_4LA_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u)(\omega) = (-i\omega)^\alpha (1 + \mathcal{O}(z^4)) \hat{u}(\omega),$$

and by the similar way to the proof of Lemma 2.3 we get

$$-_{\infty}D_x^\alpha u(x) = {}_4LA_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) + \mathcal{O}(h^4).$$

□

For the right Riemann-Liouville fractional derivative, denote that

$${}_R A_p^\alpha u(x) = \frac{1}{h^\alpha} \sum_{k=0}^{\infty} q_k^\alpha u(x + (k-p)h), \quad (2.11)$$

where  $q_k^\alpha$  is defined by (2.2) and  $p$  an integer. Using the same way as Theorems 2.1-2.3, we can obtain the following results. In particular, the coefficients in (2.12) are completely the same as the ones in (2.6); the coefficients in (2.13) the same as the ones in (2.7); and the coefficients in (2.14) the same as the ones in (2.8).

**THEOREM 2.4** (Second order approximations for right Riemann-Liouville derivative) Let  $u, {}_x D_\infty^{\alpha+2} u(x)$  with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$ , and denote that

$${}_2 R A_{p,q}^\alpha u(x) = w_p {}_R A_p^\alpha u(x) + w_q {}_R A_q^\alpha u(x), \quad (2.12)$$

then

$${}_x D_\infty^\alpha u(x) = {}_2 R A_{p,q}^\alpha u(x) + \mathcal{O}(h^2).$$

**THEOREM 2.5** (Third order approximations for right Riemann-Liouville derivative) Let  $u, {}_x D_\infty^{\alpha+3} u(x)$  with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$ , and denote that

$${}_3 R A_{p,q,r,s}^\alpha u(x) = w_{p,q} {}_2 R A_{p,q}^\alpha u(x) + w_{r,s} {}_2 R A_{r,s}^\alpha u(x), \quad (2.13)$$

then

$${}_x D_\infty^\alpha u(x) = {}_3 R A_{p,q,r,s}^\alpha u(x) + \mathcal{O}(h^3).$$

**THEOREM 2.6** (Fourth order approximations for right Riemann-Liouville derivative) Let  $u, {}_x D_\infty^{\alpha+4} u(x)$  with  $\alpha \in (1, 2)$  and their Fourier transforms belong to  $L_1(\mathbb{R})$ , and denote that

$${}_4 R A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) = w_{p,q,r,s} {}_3 R A_{p,q,r,s}^\alpha u(x) + w_{\bar{p},\bar{q},\bar{r},\bar{s}} {}_3 R A_{\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x), \quad (2.14)$$

then

$${}_x D_\infty^\alpha u(x) = {}_4 R A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) + \mathcal{O}(h^4).$$

All the above schemes are applicable to bounded domain, say,  $(x_L, x_R)$ , after performing zero extensions to the functions considered. Let  $u(x)$  be the zero extended function from the bounded domain  $(x_L, x_R)$ , and satisfy the requirements of the above corresponding theorems (Theorems 2.1-2.6). Denoting

$${}_L \tilde{A}_p^\alpha u(x) = \frac{1}{h^\alpha} \sum_{k=0}^{\lfloor \frac{x-x_L}{h} \rfloor + p} q_k^\alpha u(x - (k-p)h), \quad (2.15)$$

then

$$\begin{aligned} {}_{x_L} D_x^\alpha u(x) &= {}_L \tilde{A}_p^\alpha u(x) + \mathcal{O}(h), & p \neq 0, \\ {}_{x_L} D_x^\alpha u(x) &= {}_L \tilde{A}_p^\alpha u(x) + \mathcal{O}(h^2), & p = 0; \end{aligned} \quad (2.16)$$



$${}_{x_L}D_x^\alpha u(x) = {}_{2L}\tilde{A}_{p,q}^\alpha u(x) + \mathcal{O}(h^2), \quad \text{where } {}_{2L}\tilde{A}_{p,q}^\alpha u(x) = w_p L\tilde{A}_p^\alpha u(x) + w_q L\tilde{A}_q^\alpha u(x); \quad (2.17)$$

$${}_{x_L}D_x^\alpha u(x) = {}_{3L}\tilde{A}_{p,q,r,s}^\alpha u(x) + \mathcal{O}(h^3), \quad \text{where } {}_{3L}\tilde{A}_{p,q,r,s}^\alpha u(x) = w_{p,q} 2L\tilde{A}_{p,q}^\alpha u(x) + w_{r,s} 2L\tilde{A}_{p,q}^\alpha u(x); \quad (2.18)$$

and

$${}_{x_L}D_x^\alpha u(x) = {}_{4L}\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) + \mathcal{O}(h^4), \quad (2.19)$$

where  ${}_{4L}\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x) = w_{p,q,r,s} {}_{3L}\tilde{A}_{p,q,r,s}^\alpha u(x) + w_{\bar{p},\bar{q},\bar{r},\bar{s}} {}_{3L}\tilde{A}_{\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x)$ .

Denoting  $x_i = x_L + ih$ ,  $i = -m, \dots, 0, 1, \dots, N_x - 1, N_x, \dots, N_x + m$ , and  $h = (x_R - x_L)/N_x$  being the uniform space stepsize, it can be noted that

$$u(x_i) = 0, \quad \text{for } i = -m, -m+1, \dots, 0 \quad \text{and} \quad i = N_x, N_x+1, \dots, N_x+m,$$

where

$$m = \max(\text{abs}(p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s})). \quad (2.20)$$

Then the approximation operator of (2.15) can be described as

$$L\tilde{A}_p^\alpha u(x_i) = \frac{1}{h^\alpha} \sum_{k=0}^{i+p} q_k^\alpha u(x_{i-k+p}) = \frac{1}{h^\alpha} \sum_{k=m-p}^{i+m} q_{k+p-m}^\alpha u(x_{i-k+m}) = \frac{1}{h^\alpha} \sum_{k=0}^{i+m} q_{k+p-m}^\alpha u(x_{i-k+m}), \quad (2.21)$$

where  $q_{k+p-m}^\alpha = 0$ , when  $k+p-m < 0$ , and  $p$  is an integer. Then

$${}_{x_L}D_x^\alpha u(x_i) = L\tilde{A}_p^\alpha u(x_i) + \mathcal{O}(h) = \frac{1}{h^\alpha} \sum_{k=0}^{i+m} q_{k+p-m}^\alpha u(x_{i-k+m}) + \mathcal{O}(h), \quad p \neq 0, \quad (2.22)$$

$${}_{x_L}D_x^\alpha u(x_i) = L\tilde{A}_p^\alpha u(x_i) + \mathcal{O}(h^2) = \frac{1}{h^\alpha} \sum_{k=0}^{i+m} q_{k+p-m}^\alpha u(x_{i-k+m}) + \mathcal{O}(h^2), \quad p = 0;$$

$${}_{x_L}D_x^\alpha u(x_i) = {}_{2L}\tilde{A}_{p,q}^\alpha u(x_i) + \mathcal{O}(h^2) = \frac{1}{h^\alpha} \sum_{k=0}^{i+m} (w_p q_{k+p-m}^\alpha + w_q q_{k+q-m}^\alpha) u(x_{i-k+m}) + \mathcal{O}(h^2); \quad (2.23)$$

$$\begin{aligned} {}_{x_L}D_x^\alpha u(x_i) &= {}_{3L}\tilde{A}_{p,q,r,s}^\alpha u(x_i) + \mathcal{O}(h^3) \\ &= \frac{1}{h^\alpha} \sum_{k=0}^{i+m} (w_{p,q} w_p q_{k+p-m}^\alpha + w_{p,q} w_q q_{k+q-m}^\alpha + w_{r,s} w_r q_{k+r-m}^\alpha + w_{r,s} w_s q_{k+s-m}^\alpha) u(x_{i-k+m}) \\ &\quad + \mathcal{O}(h^3); \end{aligned} \quad (2.24)$$

$${}_{x_L}D_x^\alpha u(x_i) = {}_{4L}\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x_i) + \mathcal{O}(h^4) = \frac{1}{h^\alpha} \sum_{k=0}^{i+m} \Phi_k^\alpha u(x_{i-k+m}) + \mathcal{O}(h^4), \quad (2.25)$$

where

$$\begin{aligned} \Phi_k^\alpha &= w_{p,q,r,s} w_p w_q q_{k+p-m}^\alpha + w_{p,q,r,s} w_p w_q q_{k+q-m}^\alpha + w_{p,q,r,s} w_r w_s q_{k+r-m}^\alpha \\ &\quad + w_{p,q,r,s} w_r w_s q_{k+s-m}^\alpha + w_{\bar{p},\bar{q},\bar{r},\bar{s}} w_{\bar{p},\bar{q}} w_{\bar{p}} q_{k+\bar{p}-m}^\alpha + w_{\bar{p},\bar{q},\bar{r},\bar{s}} w_{\bar{p},\bar{q}} w_{\bar{q}} q_{k+\bar{q}-m}^\alpha \\ &\quad + w_{\bar{p},\bar{q},\bar{r},\bar{s}} w_{\bar{r},\bar{s}} w_{\bar{r}} q_{k+\bar{r}-m}^\alpha + w_{\bar{p},\bar{q},\bar{r},\bar{s}} w_{\bar{r},\bar{s}} w_{\bar{s}} q_{k+\bar{s}-m}^\alpha. \end{aligned} \quad (2.26)$$

Taking  $U = [u(x_1), u(x_2), \dots, u(x_{N_x-1})]^\top$ , then (2.21) can be rewritten as the matrix form

$$L\tilde{A}_p^\alpha U = \frac{1}{h^\alpha} A_p^\alpha U, \quad (2.27)$$



REMARK 2.1 When  $p = 0$ , then  $A_p^\alpha$  in (2.28) reduces to the lower triangular matrix, and it can be easily checked that all the eigenvalues of  $A_p^\alpha$  are greater than one; in fact, from Lemma 2.1, it can be noted that  $\lambda(A_p^\alpha) = \left(\frac{3}{2}\right)^\alpha$ , with  $\alpha \in (1, 2)$ . This is the reason that the scheme for time dependent problem is unstable when directly using the second order Lubich formula with  $\alpha \in (1, 2)$  to discretize space fractional derivative.

## 2.2 Effective fourth order discretization for space fractional derivatives

This subsection focuses on how to choose the parameters  $p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}$  such that all the eigenvalues of the matrix  $A_{p,q}^\alpha$  (or  $A_{p,q,r,s}^\alpha$  or  $A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$ ) have negative real parts; this means that the corresponding schemes work for space fractional derivatives. Since  $B_{p,q}^\alpha$ ,  $B_{p,q,r,s}^\alpha$ , and  $B_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  is, respectively, the transpose of  $A_{p,q}^\alpha$ ,  $A_{p,q,r,s}^\alpha$ , and  $A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$ , we don't need to discuss them separately.

DEFINITION 2.7 (Quarteroni *et al.*, 2007, p. 27) A matrix  $A \in \mathbb{R}^{n \times n}$  is positive definite in  $\mathbb{R}^n$  if  $(Ax, x) > 0$ ,  $\forall x \in \mathbb{R}^n, x \neq 0$ .

LEMMA 2.4 (Quarteroni *et al.*, 2007, p. 28) A real matrix  $A$  of order  $n$  is positive definite if and only if its symmetric part  $H = \frac{A+A^T}{2}$  is positive definite. Let  $H \in \mathbb{R}^{n \times n}$  be symmetric, then  $H$  is positive definite if and only if the eigenvalues of  $H$  are positive.

LEMMA 2.5 (Quarteroni *et al.*, 2007, p. 184) If  $A \in \mathbb{C}^{n \times n}$ , let  $H = \frac{A+A^H}{2}$  be the hermitian part of  $A$ , then for any eigenvalue  $\lambda$  of  $A$ , the real part  $\Re(\lambda(A))$  satisfies

$$\lambda_{\min}(H) \leq \Re(\lambda(A)) \leq \lambda_{\max}(H),$$

where  $\lambda_{\min}(H)$  and  $\lambda_{\max}(H)$  are the minimum and maximum of the eigenvalues of  $H$ , respectively.

DEFINITION 2.8 (Chan & Jin, 2007, p. 13) Let  $n \times n$  Toeplitz matrix  $T_n$  be of the following form:

$$T_n = \begin{bmatrix} t_0 & t_{-1} & \cdots & t_{2-n} & t_{1-n} \\ t_1 & t_0 & t_{-1} & \cdots & t_{2-n} \\ \vdots & t_1 & t_0 & \ddots & \vdots \\ t_{n-2} & \cdots & \ddots & \ddots & t_{-1} \\ t_{n-1} & t_{n-2} & \cdots & t_1 & t_0 \end{bmatrix};$$

i.e.,  $t_{i,j} = t_{i-j}$  and  $T_n$  is constant along its diagonals. Assume that the diagonals  $\{t_k\}_{k=-n+1}^{n-1}$  are the Fourier coefficients of a function  $f$ , i.e.,

$$t_k = \frac{1}{2\pi} \int_{-\pi}^{\pi} f(x) e^{-ikx} dx,$$

then the function  $f$  is called the generating function of  $T_n$ .

LEMMA 2.6 (Chan & Jin, 2007, p. 13-15) (Grenander-Szegö theorem) Let  $T_n$  be given by above matrix with a generating function  $f$ , where  $f$  is a  $2\pi$ -periodic continuous real-valued functions defined on  $[-\pi, \pi]$ . Let  $\lambda_{\min}(T_n)$  and  $\lambda_{\max}(T_n)$  denote the smallest and largest eigenvalues of  $T_n$ , respectively. Then we have

$$f_{\min} \leq \lambda_{\min}(T_n) \leq \lambda_{\max}(T_n) \leq f_{\max},$$

where  $f_{min}$  and  $f_{max}$  is the minimum and maximum values of  $f(x)$ , respectively. Moreover, if  $f_{min} < f_{max}$ , then all eigenvalues of  $T_n$  satisfies

$$f_{min} < \lambda(T_n) < f_{max},$$

for all  $n > 0$ ; In particular, if  $f_{min} > 0$ , then  $T_n$  is positive definite.

**THEOREM 2.9** (Effective second order schemes) Let  $A_{p,q}^\alpha$  be given in (2.29) and  $1 < \alpha < 2$ . Then any eigenvalue  $\lambda$  of  $A_{p,q}^\alpha$  satisfies

$$\Re(\lambda(A_{p,q}^\alpha)) < 0 \quad \text{for } (p,q) = (1,q), \quad |q| \geq 2,$$

moreover, the matrices  $A_{p,q}^\alpha$  and  $(A_{p,q}^\alpha)^T$  are negative definite.

*Proof.*

(1) For  $(p,q) = (1,q)$ ,  $q \leq -2$ , we have  $A_{p,q}^\alpha = \frac{1}{q-1}(qA_1^\alpha - A_q^\alpha)$ , and

$$A_{p,q}^\alpha = \begin{bmatrix} \phi_1^\alpha & \phi_0^\alpha & & & \\ \phi_2^\alpha & \phi_1^\alpha & \phi_0^\alpha & & \\ \vdots & \ddots & \ddots & \ddots & \\ \phi_{N_x-2}^\alpha & \ddots & \ddots & \phi_1^\alpha & \phi_0^\alpha \\ \phi_{N_x-1}^\alpha & \phi_{N_x-2}^\alpha & \cdots & \phi_2^\alpha & \phi_1^\alpha \end{bmatrix},$$

with

$$\phi_k^\alpha = \begin{cases} \frac{qq_k^\alpha}{q-1}, & 0 \leq k \leq -q, \\ \frac{qq_k^\alpha - q_{k+q-1}^\alpha}{q-1}, & k > -q. \end{cases}$$

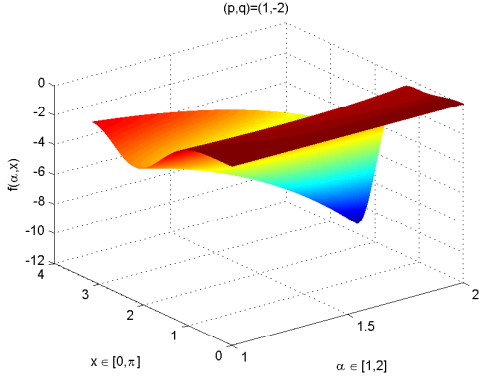
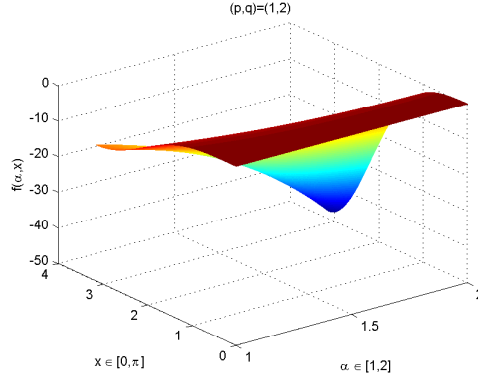
The generating functions of  $A_{p,q}^\alpha$  and  $(A_{p,q}^\alpha)^T$  are

$$f_{A_{p,q}^\alpha}(x) = \sum_{k=0}^{\infty} \phi_k^\alpha e^{i(k-1)x} \quad \text{and} \quad f_{(A_{p,q}^\alpha)^T}(x) = \sum_{k=0}^{\infty} \phi_k^\alpha e^{-i(k-1)x},$$

respectively. Taking  $H_{p,q} = \frac{A_{p,q}^\alpha + (A_{p,q}^\alpha)^T}{2}$ , then  $f_{p,q}(\alpha, x) = \frac{f_{A_{p,q}^\alpha}(x) + f_{(A_{p,q}^\alpha)^T}(x)}{2}$  is the generating function of  $H_{p,q}$ . Since  $f_{A_{p,q}^\alpha}(x)$  and  $f_{(A_{p,q}^\alpha)^T}(x)$  are mutually conjugated, then  $f_{p,q}(\alpha, x)$  is a  $2\pi$ -periodic continuous real-valued functions defined on  $[-\pi, \pi]$ . Moreover,  $f_{p,q}(\alpha, x)$  is an even function, so we just need to consider its principal value on  $[0, \pi]$ . Next, we prove  $f_{p,q}(\alpha, x) \leq 0$ . Rephrasing the generating function leads to

$$\begin{aligned} f_{p,q}(\alpha, x) &= \frac{1}{2} \left( \sum_{k=0}^{\infty} \phi_k^\alpha e^{i(k-1)x} + \sum_{k=0}^{\infty} \phi_k^\alpha e^{-i(k-1)x} \right) \\ &= \frac{1}{2(q-1)} \left( qe^{-ix} \sum_{k=0}^{\infty} q_k^\alpha e^{ikx} - e^{-iqx} \sum_{k=0}^{\infty} q_k^\alpha e^{ikx} + qe^{ix} \sum_{k=0}^{\infty} q_k^\alpha e^{-ikx} - e^{iqx} \sum_{k=0}^{\infty} q_k^\alpha e^{-ikx} \right) \\ &= \frac{1}{2(q-1)} \left[ qe^{-ix}(1-e^{ix})^\alpha \left( 1 + \frac{1}{2}(1-e^{ix}) \right)^\alpha + qe^{ix}(1-e^{-ix})^\alpha \left( 1 + \frac{1}{2}(1-e^{-ix}) \right)^\alpha \right] \\ &\quad - \frac{1}{2(q-1)} \left[ e^{-iqx}(1-e^{ix})^\alpha \left( 1 + \frac{1}{2}(1-e^{ix}) \right)^\alpha + e^{iqx}(1-e^{-ix})^\alpha \left( 1 + \frac{1}{2}(1-e^{-ix}) \right)^\alpha \right]. \end{aligned}$$



FIG. 1.  $f(\alpha, x)$  for  $(p, q) = (1, -2)$ FIG. 2.  $f(\alpha, x) \leq 0$  for  $(p, q) = (1, 2)$ 

It can be noted that  $f_{p,q}(\alpha, x)$  has the same form when  $q \leq -2$  and  $q \geq 2$ ,  $p = 1$ . And we can check that, for  $(p, q) = (1, q)$ ,  $|q| \geq 2$ , there exists (see Figs. 1-2)

$$f_{p,q}(\alpha, x) = \frac{1}{q-1} \left(2\sin\frac{x}{2}\right)^\alpha \left(1 + 3\sin^2\frac{x}{2}\right)^{\frac{\alpha}{2}} \cdot \left[q\cos\left(\alpha\left(x - \frac{\pi}{2} - \theta\right) - x\right) - \cos\left(\alpha\left(x - \frac{\pi}{2} - \theta\right) - qx\right)\right] \leq 0. \quad (2.35)$$

Since  $f_{p,q}(\alpha, x)$  is not identically zero for any given  $\alpha \in (1, 2)$ , from Lemma 2.6, it implies that  $\lambda(H_{p,q}) < 0$  and  $H_{p,q}$  is negative definite. Then we get  $\Re(\lambda(A_{p,q}^\alpha)) < 0$  from Lemma 2.5, and the matrices  $A_{p,q}^\alpha$  and  $(A_{p,q}^\alpha)^T$  are negative definite by Lemma 2.4.  $\square$

**THEOREM 2.10** (Effective third order schemes) Let  $A_{p,q,r,s}^\alpha$  with  $1 < \alpha < 2$  be given in (2.30). Then any eigenvalue  $\lambda$  of  $A_{p,q,r,s}^\alpha$  satisfies

$$\Re(\lambda(A_{p,q,r,s}^\alpha)) < 0 \quad \text{for } (p, q, r, s) = (1, q, 1, s), \quad |q| \geq 2, \quad |s| \geq 2, \quad \text{and } qs < 0;$$

moreover, the matrices  $A_{p,q,r,s}^\alpha$  and  $(A_{p,q,r,s}^\alpha)^T$  are negative definite.

*Proof.* Taking

$$H_{p,q,r,s} = \frac{A_{p,q,r,s}^\alpha + (A_{p,q,r,s}^\alpha)^T}{2} = w_{p,q}H_{p,q} + w_{r,s}H_{r,s}, \quad (2.36)$$

where  $H_{p,q}$  and  $H_{r,s}$  are defined by (2.34), then

$$f_{p,q,r,s}(\alpha, x) = w_{p,q}f_{p,q}(\alpha, x) + w_{r,s}f_{r,s}(\alpha, x) \quad (2.37)$$

is the generating function of  $H_{p,q,r,s}$ , where  $f_{p,q}(\alpha, x)$  and  $f_{r,s}(\alpha, x)$  are given by (2.35). Since  $|q| \geq 2$ ,  $|s| \geq 2$ , and  $qs < 0$ , we can check that  $w_{p,q} = w_{1,q} = \frac{3s+2\alpha}{3(s-q)} > 0$ ,  $w_{r,s} = w_{1,s} = \frac{3q+2\alpha}{3(q-s)} > 0$ . Then from (2.35) and (2.37), we get  $f_{p,q,r,s}(\alpha, x) \leq 0$ .

Again, from Lemmas 2.4-2.6, the desired results are obtained.  $\square$

**THEOREM 2.11** (Effective fourth order schemes) Let  $A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  with  $1 < \alpha < 2$  be given in (2.31), where  $(p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) = (1, 2, 1, -2, 1, \bar{q}, 1, \bar{s})$ ,  $|\bar{q}| \geq 2$ ,  $|\bar{s}| \geq 2$ ,  $(\bar{q}, \bar{s}) \neq (2, -2)$  and  $\bar{q}\bar{s} < 0$ . Then any eigenvalue  $\lambda$  of  $A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  satisfies

$$\Re(\lambda(A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha)) < 0,$$

and the matrices  $A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  and  $(A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha)^T$  are negative definite.

Moreover, if  $(p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s})$  takes the following values

$$\begin{aligned} (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, 2, 1, 0, 1, 2, 1, -2), \\ (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, 2, 1, 0, 1, -1, 1, -2), \\ (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, 2, 1, -1, 1, 2, 1, -2), \\ (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, 2, 1, -1, 1, -1, 1, -2), \\ (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, 0, 1, -1, 1, 2, 1, -2), \\ (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, 0, 1, -2, 1, 2, 1, -2), \\ (p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s}) &= (1, -1, 1, -2, 1, 2, 1, -2), \end{aligned}$$

then  $\Re(\lambda(A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha)) < 0$  and the matrices  $A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  and  $(A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha)^T$  are negative definite.

*Proof.* By the similar way to the proofs of Theorems 2.9 and 2.10, we obtain the desired results.  $\square$

### 3. Application to the space fractional diffusion equations: the one dimensional case of (1.2) and (1.2) itself

We use two subsections to derive the full discretization of (1.2). First, we present the scheme for the one dimensional case of (1.2). The second subsection detailedly provides the full discrete scheme of the two-dimensional fractional diffusion equation (1.2) with variable coefficients.

#### 3.1 Numerical scheme for 1D

In this subsection, we consider the one-dimensional case of (1.2) with variable coefficients, namely,

$$\frac{\partial u(x, t)}{\partial t} = d_+(x)_{x_L} D_x^\alpha u(x, t) + d_-(x)_{x_R} D_{x_R}^\alpha u(x, t) + f(x, t). \quad (3.1)$$

In the time direction, we use the Crank-Nicolson scheme. The fourth order left fractional approximation operator (2.25), and right fractional approximation operator (2.32) are respectively used to discretize the left Riemann-Liouville fractional derivative, and right Riemann-Liouville fractional derivative.

Let the mesh points  $x_i = x_L + ih$ ,  $i = -m, \dots, 0, 1, \dots, N_x - 1, N_x, \dots, N_x + m$ , where  $m$  is defined by (2.20) and  $t_n = n\tau$ ,  $0 \leq n \leq N_t$ , where  $h = (x_R - x_L)/N_x$ ,  $\tau = T/N_t$ , i.e.,  $h$  is the uniform space stepsize and  $\tau$  the time steplength. Taking  $u_i^n$  as the approximated value of  $u(x_i, t_n)$  and  $d_{+,i} = d_+(x_i)$ ,  $d_{-,i} = d_-(x_i)$ ,  $f_i^{n+1/2} = f(x_i, t_{n+1/2})$ , where  $t_{n+1/2} = (t_n + t_{n+1})/2$ . Then, Eq. (3.1) can be rewritten as

$$\begin{aligned} \frac{u(x_i, t_{n+1}) - u(x_i, t_n)}{\tau} &= \frac{1}{2} \left[ d_{+,i} {}_4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x_i, t_{n+1}) + d_{+,i} {}_4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x_i, t_n) \right. \\ &\quad \left. + d_{-,i} {}_4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x_i, t_{n+1}) + d_{-,i} {}_4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha u(x_i, t_n) \right] \\ &\quad + f(x_i, t_{n+1/2}) + \mathcal{O}(\tau^2 + h^4). \end{aligned} \quad (3.2)$$

16 of 24

Multiplying (3.2) by  $\tau$ , we have the following equation

$$\begin{aligned} & \left[ 1 - \frac{\tau}{2} \left( d_{+,i} 4L \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha \right) \right] u(x_i, t_{n+1}) \\ & = \left[ 1 + \frac{\tau}{2} \left( d_{+,i} 4L \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha \right) \right] u(x_i, t_n) + \tau f(x_i, t_{n+1/2}) + R_i^{n+1}, \end{aligned} \quad (3.3)$$

with

$$|R_i^{n+1}| \leq \tilde{c}\tau(\tau^2 + h^4). \quad (3.4)$$

Therefore, the full discretization of (3.3) has the following form

$$\begin{aligned} & \left[ 1 - \frac{\tau}{2} \left( d_{+,i} 4L \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha \right) \right] u_i^{n+1} \\ & = \left[ 1 + \frac{\tau}{2} \left( d_{+,i} 4L \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R \tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha \right) \right] u_i^n + \tau f_i^{n+1/2}, \end{aligned} \quad (3.5)$$

and it can be rewritten as

$$\begin{aligned} & u_i^{n+1} - \frac{\tau}{2} \left[ \frac{d_{+,i}}{h^\alpha} \sum_{k=0}^{i+m} \varphi_k^\alpha u_{i-k+m}^{n+1} + \frac{d_{-,i}}{h^\alpha} \sum_{k=0}^{N_x-i+m} \varphi_k^\alpha u_{i+k-m}^{n+1} \right] \\ & = u_i^n + \frac{\tau}{2} \left[ \frac{d_{+,i}}{h^\alpha} \sum_{k=0}^{i+m} \varphi_k^\alpha u_{i-k+m}^n + \frac{d_{-,i}}{h^\alpha} \sum_{k=0}^{N_x-i+m} \varphi_k^\alpha u_{i+k-m}^n \right] + \tau f_i^{n+1/2}. \end{aligned} \quad (3.6)$$

For the convenience of implementation, we use the matrix form of the grid functions

$$U^n = [u_1^n, u_2^n, \dots, u_{N_x-1}^n]^\top, \quad F^{n+1/2} = [f_1^{n+1/2}, f_2^{n+1/2}, \dots, f_{N_x-1}^{n+1/2}]^\top,$$

therefore, the finite difference scheme (3.6) can be recast as

$$\left[ I - \frac{\tau}{2h^\alpha} (D_+ A_\alpha + D_- A_\alpha^\top) \right] U^{n+1} = \left[ I + \frac{\tau}{2h^\alpha} (D_+ A_\alpha + D_- A_\alpha^\top) \right] U^n + \tau F^{n+1/2}, \quad (3.7)$$

where  $A_\alpha = A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  is defined by (2.31), and

$$D_+ = \begin{bmatrix} d_{+,1} & & & \\ & d_{+,2} & & \\ & & \ddots & \\ & & & d_{+,N_x-1} \end{bmatrix}, \quad D_- = \begin{bmatrix} d_{-,1} & & & \\ & d_{-,2} & & \\ & & \ddots & \\ & & & d_{-,N_x-1} \end{bmatrix}. \quad (3.8)$$

### 3.2 Numerical scheme for 2D

We now examine the full discretization scheme of (1.2). For effectively performing the theoretical analysis, we suppose  $d_+(x) = d_+(x, y)$ ,  $d_-(x) = d_-(x, y)$ , and  $e_+(y) = e_+(x, y)$ ,  $e_-(y) = e_-(x, y)$ .

Analogously we still use the Crank-Nicolson scheme to do the discretization in time direction. Let the mesh points  $x_i = x_L + ih$ ,  $i = -m, \dots, 0, 1, \dots, N_x - 1, N_x, \dots, N_x + m$ , and  $y_j = y_L + j\Delta y$ ,  $j = -m, \dots, 0, 1, \dots, N_y - 1, N_y, \dots, N_y + m$ , where  $m$  is given in (2.20),  $t_n = n\tau$ ,  $0 \leq n \leq N_t$ , and  $\Delta x = (x_R - x_L)/N_x$ ,  $\Delta y = (y_R - y_L)/N_y$ ,  $\tau = T/N_t$ ; and  $d_{+,i} = d_+(x_i, y_j)$ ,  $d_{-,i} = d_-(x_i, y_j)$ , and  $e_{+,j} = e_+(x_i, y_j)$ ,



$e_{-,j} = e_-(x_i, y_j)$ . Taking  $u_{i,j}^n$  as the approximated value of  $u(x_i, y_j, t_n)$  and  $f_{i,j}^{n+1/2} = f(x_i, y_j, t_{n+1/2})$ , where  $t_{n+1/2} = (t_n + t_{n+1})/2$ . Then, Eq. (1.2) can be rewritten as

$$\begin{aligned} & \left[ 1 - \frac{\tau}{2} \left( d_{+,i} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + e_{+,j} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta + e_{-,j} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta \right) \right] u(x_i, y_j, t_{n+1}) \\ &= \left[ 1 + \frac{\tau}{2} \left( d_{+,i} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + e_{+,j} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta + e_{-,j} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta \right) \right] u(x_i, y_j, t_n) \\ & \quad + \tau f(x_i, y_j, t_{n+1/2}) + R_{i,j}^{n+1}, \end{aligned} \quad (3.9)$$

with

$$|R_{i,j}^{n+1}| \leq \tilde{c}\tau(\tau^2 + (\Delta x)^4 + (\Delta y)^4). \quad (3.10)$$

Then, the resulting discretization of (3.9) has the following form

$$\begin{aligned} & \left[ 1 - \frac{\tau}{2} \left( d_{+,i} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + e_{+,j} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta + e_{-,j} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta \right) \right] u_{i,j}^{n+1} \\ &= \left[ 1 + \frac{\tau}{2} \left( d_{+,i} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + e_{+,j} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta + e_{-,j} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta \right) \right] u_{i,j}^n \\ & \quad + \tau f_{i,j}^{n+1/2}. \end{aligned} \quad (3.11)$$

We further define

$$\begin{aligned} \delta_{\alpha,x} &:= d_{+,i} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha + d_{-,i} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha; \\ \delta_{\beta,y} &:= e_{+,j} 4L\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta + e_{-,j} 4R\tilde{A}_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta, \end{aligned}$$

thus Eq. (3.11) can be rewritten as

$$\left( 1 - \frac{\tau}{2} \delta_{\alpha,x} - \frac{\tau}{2} \delta_{\beta,y} \right) u_{i,j}^{n+1} = \left( 1 + \frac{\tau}{2} \delta_{\alpha,x} + \frac{\tau}{2} \delta_{\beta,y} \right) u_{i,j}^n + \tau f_{i,j}^{n+1/2}. \quad (3.12)$$

The perturbation equation of (3.12) is of the form

$$\left( 1 - \frac{\tau}{2} \delta_{\alpha,x} \right) \left( 1 - \frac{\tau}{2} \delta_{\beta,y} \right) u_{i,j}^{n+1} = \left( 1 + \frac{\tau}{2} \delta_{\alpha,x} \right) \left( 1 + \frac{\tau}{2} \delta_{\beta,y} \right) u_{i,j}^n + \tau f_{i,j}^{n+1/2}. \quad (3.13)$$

Comparing (3.13) with (3.12), the splitting term is given by

$$\frac{\tau^2}{4} \delta_{\alpha,x} \delta_{\beta,y} (u_{i,j}^{n+1} - u_{i,j}^n),$$

since  $(u_{i,j}^{n+1} - u_{i,j}^n)$  is an  $\mathcal{O}(\tau)$  term, it implies that this perturbation contributes an  $\mathcal{O}(\tau^2)$  error component.

The system of equations defined by (3.13) can be solved by the following schemes.

PR-ADI scheme [Peaceman & Rachford (1955)]:

$$\left( 1 - \frac{\tau}{2} \delta_{\alpha,x} \right) u_{i,j}^* = \left( 1 + \frac{\tau}{2} \delta_{\beta,y} \right) u_{i,j}^n + \frac{\tau}{2} f_{i,j}^{n+1/2}; \quad (3.14)$$

$$\left(1 - \frac{\tau}{2}\delta_{\beta,y}\right)u_{i,j}^{n+1} = \left(1 + \frac{\tau}{2}\delta_{\alpha,x}\right)u_{i,j}^* + \frac{\tau}{2}f_{i,j}^{n+1/2}. \quad (3.15)$$

D-ADI scheme [Dougl's (1955)]:

$$\left(1 - \frac{\tau}{2}\delta_{\alpha,x}\right)u_{i,j}^* = \left(1 + \frac{\tau}{2}\delta_{\alpha,x} + \tau\delta_{\beta,y}\right)u_{i,j}^n + \tau f_{i,j}^{n+1/2}; \quad (3.16)$$

$$\left(1 - \frac{\tau}{2}\delta_{\beta,y}\right)u_{i,j}^{n+1} = u_{i,j}^* - \frac{\tau}{2}\delta_{\beta,y}u_{i,j}^n. \quad (3.17)$$

Take

$$\begin{aligned} \mathbf{U}^n &= [u_{1,1}^n, u_{2,1}^n, \dots, u_{N_x-1,1}^n, u_{1,2}^n, u_{2,2}^n, \dots, u_{N_x-1,2}^n, \dots, u_{1,N_y-1}^n, u_{2,N_y-1}^n, \dots, u_{N_x-1,N_y-1}^n]^T, \\ \mathbf{F}^n &= [f_{1,1}^n, f_{2,1}^n, \dots, f_{N_x-1,1}^n, f_{1,2}^n, f_{2,2}^n, \dots, f_{N_x-1,2}^n, \dots, f_{1,N_y-1}^n, f_{2,N_y-1}^n, \dots, f_{N_x-1,N_y-1}^n]^T, \end{aligned}$$

and denote

$$\begin{aligned} \mathcal{A}_x &= \frac{\tau}{2(\Delta x)^\alpha} [(I \otimes D_+)(I \otimes A_\alpha) + (I \otimes D_-)(I \otimes A_\alpha^T)] = \frac{\tau}{2(\Delta x)^\alpha} I \otimes (D_+ A_\alpha + D_- A_\alpha^T), \\ \mathcal{A}_y &= \frac{\tau}{2(\Delta y)^\beta} [(E_+ \otimes I)(A_\beta \otimes I) + (E_- \otimes I)(A_\beta^T \otimes I)] = \frac{\tau}{2(\Delta y)^\beta} (E_+ A_\beta + E_- A_\beta^T) \otimes I, \end{aligned} \quad (3.18)$$

where  $I$  denotes the unit matrix and the symbol  $\otimes$  the Kronecker product [see, Laub (2005)], and  $A_\alpha = A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$ ,  $A_\beta = A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\beta$  are defined by (2.31). The matrices  $D_+$  and  $D_-$  are defined by (3.8), and

$$E_+ = \begin{bmatrix} e_{+,1} & & & & \\ & e_{+,2} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & e_{+,N_y-1} \end{bmatrix}, \quad E_- = \begin{bmatrix} e_{-,1} & & & & \\ & e_{-,2} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & e_{-,N_y-1} \end{bmatrix}. \quad (3.19)$$

Therefore, the finite difference scheme (3.13) has the following form

$$(I - \mathcal{A}_x)(I - \mathcal{A}_y)\mathbf{U}^{n+1} = (I + \mathcal{A}_x)(I + \mathcal{A}_y)\mathbf{U}^n + \tau\mathbf{F}^{n+1/2}. \quad (3.20)$$

**REMARK 3.1** The schemes (3.14)-(3.15) and (3.16)-(3.17) are equivalent, since both of them come from (3.13), see [Deng & Chen (2013)].

#### 4. Convergence and Stability Analysis

In this section, we theoretically prove that the difference scheme is unconditionally stable and 4th order convergent in space directions and 2nd order convergent in time direction. In the following, the matrices  $D_+$ ,  $D_-$  and  $E_+$ ,  $E_-$  are defined by (3.8) and (3.19), respectively.

**LEMMA 4.1** (Laub, 2005, p. 140) Let  $A \in \mathbb{R}^{m \times n}$ ,  $B \in \mathbb{R}^{r \times s}$ ,  $C \in \mathbb{R}^{n \times p}$ , and  $D \in \mathbb{R}^{s \times t}$ . Then

$$(A \otimes B)(C \otimes D) = AC \otimes BD \quad (\in \mathbb{R}^{mr \times pt}).$$

Moreover, for all  $A$  and  $B$ ,  $(A \otimes B)^T = A^T \otimes B^T$ .

LEMMA 4.2 (Laub, 2005, p. 141) Let  $A \in \mathbb{R}^{n \times n}$  have eigenvalues  $\{\lambda_i\}_{i=1}^n$  and  $B \in \mathbb{R}^{m \times m}$  have eigenvalues  $\{\mu_j\}_{j=1}^m$ . Then the  $mn$  eigenvalues of  $A \otimes B$  are

$$\lambda_1 \mu_1, \dots, \lambda_1 \mu_m, \lambda_2 \mu_1, \dots, \lambda_2 \mu_m, \dots, \lambda_n \mu_1, \dots, \lambda_n \mu_m.$$

THEOREM 4.1 Let the matrix  $A_\alpha = A_{p,q,r,s,\bar{p},\bar{q},\bar{r},\bar{s}}^\alpha$  be defined by (2.31) and  $D_- = \kappa_\alpha D_+$ , where  $\kappa_\alpha$  is any given nonnegative constant. Then we have  $\Re(\lambda(D_+(A_\alpha + \kappa_\alpha A_\alpha^T))) < 0$ .

*Proof.* Since

$$D_+^{-\frac{1}{2}} [D_+(A_\alpha + \kappa_\alpha A_\alpha^T)] D_+^{\frac{1}{2}} = D_+^{\frac{1}{2}} (A_\alpha + \kappa_\alpha A_\alpha^T) D_+^{\frac{1}{2}},$$

it means that  $D_+(A_\alpha + \kappa_\alpha A_\alpha^T)$  and  $D_+^{\frac{1}{2}} (A_\alpha + \kappa_\alpha A_\alpha^T) D_+^{\frac{1}{2}}$  are similar. From Theorem 2.11, we know  $A_\alpha$  and  $A_\alpha^T$  are negative definite, and thanks to Definition 2.7, it implies that

$$\left( D_+^{\frac{1}{2}} (A_\alpha + \kappa_\alpha A_\alpha^T) D_+^{\frac{1}{2}} x, x \right) = \left( (A_\alpha + \kappa_\alpha A_\alpha^T) D_+^{\frac{1}{2}} x, D_+^{\frac{1}{2}} x \right) < 0, \quad \forall x \in \mathbb{R}^n, x \neq 0,$$

i.e., the matrix  $\tilde{A} := D_+^{\frac{1}{2}} (A_\alpha + \kappa_\alpha A_\alpha^T) D_+^{\frac{1}{2}}$  is negative definite. From Lemma 2.4,  $\tilde{H} = \frac{\tilde{A} + \tilde{A}^T}{2}$  is negative definite and  $\lambda_{\max}(\tilde{H}) < 0$ ; and according to Lemma 2.5, we obtain  $\Re(\lambda(\tilde{A})) \leq \lambda_{\max}(\tilde{H}) < 0$ . Therefore,  $\Re(\lambda(D_+(A_\alpha + \kappa_\alpha A_\alpha^T))) = \Re(\lambda(\tilde{A})) < 0$ .  $\square$

THEOREM 4.2 Let  $\mathcal{A}_x$  and  $\mathcal{A}_y$  be defined by (3.18) and  $D_- = \kappa_\alpha D_+$ ,  $E_- = \kappa_\beta E_+$ , where  $\kappa_\alpha$  and  $\kappa_\beta$  are any given nonnegative constants. Then we have  $\Re(\lambda(\mathcal{A}_x)) < 0$  and  $\Re(\lambda(\mathcal{A}_y)) < 0$ .

*Proof.* From (3.18), there exists

$$\begin{aligned} \mathcal{A}_x &= \frac{\tau}{2(\Delta x)^\alpha} I \otimes (D_+ A_\alpha + D_- A_\alpha^T) = \frac{\tau}{2(\Delta x)^\alpha} I \otimes (D_+(A_\alpha + \kappa_\alpha A_\alpha^T)), \\ \mathcal{A}_y &= \frac{\tau}{2(\Delta y)^\beta} (E_+ A_\beta + E_- A_\beta^T) \otimes I = \frac{\tau}{2(\Delta y)^\beta} (E_+(A_\beta + \kappa_\beta A_\beta^T)) \otimes I. \end{aligned}$$

By Theorem 4.1, we get  $\Re(\lambda(D_+(A_\alpha + \kappa_\alpha A_\alpha^T))) < 0$  and  $\Re(\lambda(E_+(A_\beta + \kappa_\beta A_\beta^T))) < 0$ . Then, according to Lemma 4.2, it implies that  $\Re(\lambda(\mathcal{A}_x)) < 0$  and  $\Re(\lambda(\mathcal{A}_y)) < 0$ .  $\square$

REMARK 4.1 If taking  $\kappa_\alpha = \kappa_\beta = 0$ , then Eq. (1.2) becomes the one-sided fractional diffusion equation; and  $\kappa_\alpha = \kappa_\beta = 1$ , Eq. (1.2) reduces to the space-Riesz fractional diffusion equation.

#### 4.1 Stability and Convergence for 1D

THEOREM 4.3 Let  $D_- = \kappa_\alpha D_+$ , then the difference scheme (3.7) with  $\alpha \in (1, 2)$  is unconditionally stable.

*Proof.* Let  $\tilde{u}_i^n$  ( $i = 1, 2, \dots, N_x - 1$ ;  $n = 0, 1, \dots, N_t$ ) be the approximate solution of  $u_i^n$ , which is the exact solution of the difference scheme (3.7). Putting  $\varepsilon_i^n = \tilde{u}_i^n - u_i^n$ , and denoting  $\varepsilon^n = [\varepsilon_1^n, \varepsilon_2^n, \dots, \varepsilon_{N_x-1}^n]$ , then from (3.7) we obtain the following perturbation equation

$$(I - A)\varepsilon^{n+1} = (I + A)\varepsilon^n,$$

i.e.,

$$\varepsilon^{n+1} = (I - A)^{-1}(I + A)\varepsilon^n,$$

with

$$A = \frac{\tau}{2h\alpha} D_+(A_\alpha + \kappa_\alpha A_\alpha^T). \quad (4.1)$$

Denoting  $\lambda$  as an eigenvalue of the matrix  $A$ , then from Theorem 4.1, we get  $\Re(\lambda(A)) < 0$ . Note that  $\lambda$  is an eigenvalue of the matrix  $A$  if and only if  $1 - \lambda$  is an eigenvalue of the matrix  $I - A$ , if and only if  $(1 - \lambda)^{-1}(1 + \lambda)$  is an eigenvalue of the matrix  $(I - A)^{-1}(I + A)$ . Since  $\Re(\lambda(A)) < 0$ , it implies that  $|(1 - \lambda)^{-1}(1 + \lambda)| < 1$ . Thus, the spectral radius of the matrix  $(I - A)^{-1}(I + A)$  is less than 1, hence the scheme (3.7) is unconditionally stable.  $\square$

**THEOREM 4.4** Let  $u(x_i, t_n)$  be the exact solution of (3.1) with  $\alpha \in (1, 2)$ ,  $u_i^n$  the solution of the finite difference scheme (3.7), and  $D_- = \kappa_\alpha D_+$ , then there is a positive constant  $C$  such that

$$\|u(x_i, t_n) - u_i^n\|_2 \leq C(\tau^2 + h^4), \quad i = 1, 2, \dots, N_x - 1; n = 0, 1, \dots, N_t.$$

*Proof.* Denoting  $e_i^n = u(x_i, t_n) - u_i^n$ , and  $e^n = [e_1^n, e_2^n, \dots, e_{N_x-1}^n]^T$ . Subtracting (3.2) from (3.7) and using  $e^0 = 0$ , we obtain

$$(I - A)e^{n+1} = (I + A)e^n + R^{n+1},$$

where  $A$  is defined by (4.1), and  $R^n = [R_1^n, R_2^n, \dots, R_{N_x-1}^n]^T$ . The above equation can be rewritten as

$$e^{n+1} = (I - A)^{-1}(I + A)e^n + (I - A)^{-1}R^{n+1}.$$

Similar to the proof of Theorem 4.2 of [Deng & Chen (2013)], we have that  $\|(I - A)^{-1}(I + A)\|_2$  and  $\|(I - A)^{-1}\|_2$  are less than 1. Then, using  $|R_i^{n+1}| \leq \tilde{c}\tau(\tau^2 + h^4)$  in (3.4), we obtain

$$\begin{aligned} \|e^n\|_2 &\leq \|(I - A)^{-1}(I + A)\|_2 \cdot \|e^{n-1}\|_2 + \|(I - A)^{-1}\|_2 \cdot |R^n| \\ &\leq \|e^{n-1}\|_2 + |R^n| \leq \sum_{k=0}^{n-1} |R^{k+1}| \leq c(\tau^2 + h^4). \end{aligned}$$

$\square$

#### 4.2 Stability and Convergence for 2D

**THEOREM 4.5** Let  $D_- = \kappa_\alpha D_+$  and  $E_- = \kappa_\beta E_+$ , then the difference scheme (3.20) with  $1 < \alpha, \beta < 2$  is unconditionally stable.

*Proof.* Let  $\tilde{u}_{i,j}^n$  ( $i = 1, 2, \dots, N_x - 1; j = 1, 2, \dots, N_y - 1; n = 0, 1, \dots, N_t$ ) be the approximate solution of  $u_{i,j}^n$ , which is the exact solution of the difference scheme (3.20). Taking  $\epsilon_{i,j}^n = \tilde{u}_{i,j}^n - u_{i,j}^n$ , then from (3.20) we obtain the following perturbation equation

$$(I - \mathcal{A}_x)(I - \mathcal{A}_y)\boldsymbol{\epsilon}^{n+1} = (I + \mathcal{A}_x)(I + \mathcal{A}_y)\boldsymbol{\epsilon}^n, \quad (4.2)$$

where  $\mathcal{A}_x$  and  $\mathcal{A}_y$  are given by (3.18), and

$$\boldsymbol{\epsilon}^n = [\epsilon_{1,1}^n, \epsilon_{2,1}^n, \dots, \epsilon_{N_x-1,1}^n, \epsilon_{1,2}^n, \epsilon_{2,2}^n, \dots, \epsilon_{N_x-1,2}^n, \dots, \epsilon_{1,N_y-1}^n, \epsilon_{2,N_y-1}^n, \dots, \epsilon_{N_x-1,N_y-1}^n]^T.$$

Then Eq. (4.2) can be rewritten as

$$\boldsymbol{\epsilon}^{n+1} = (I - \mathcal{A}_y)^{-1}(I - \mathcal{A}_x)^{-1}(I + \mathcal{A}_x)(I + \mathcal{A}_y)\boldsymbol{\epsilon}^n. \quad (4.3)$$

According to Lemma 4.1 and (3.18), it is easy to check that  $\mathcal{A}_x$  and  $\mathcal{A}_y$  commute, i.e.,

$$\mathcal{A}_x \mathcal{A}_y = \mathcal{A}_y \mathcal{A}_x = \frac{\tau^2}{4(\Delta x)^\alpha (\Delta y)^\beta} \left( E_+ A_\beta + E_- A_\beta^T \right) \otimes (D_+ A_\alpha + D_- A_\alpha^T). \quad (4.4)$$

Then Eq. (4.3) has the following form

$$\mathbf{e}^{n+1} = (I - \mathcal{A}_x)^{-1} (I + \mathcal{A}_x) (I - \mathcal{A}_y)^{-1} (I + \mathcal{A}_y) \mathbf{e}^n. \quad (4.5)$$

Form Theorem 4.2, we have  $\Re(\lambda(\mathcal{A}_x)) < 0$  and  $\Re(\lambda(\mathcal{A}_y)) < 0$ . Similar to the proof of the Theorem 4.3, the spectral radius of the matrix  $(I - \mathcal{A}_x)^{-1} (I + \mathcal{A}_x)$  and  $(I - \mathcal{A}_y)^{-1} (I + \mathcal{A}_y)$  are less than 1. Then the difference scheme (3.20) is unconditionally stable.  $\square$

**THEOREM 4.6** Let  $u(x_i, y_j, t_n)$  be the exact solution of (1.2) with  $1 < \alpha, \beta < 2$ ,  $u_{i,j}^n$  the solution of the finite difference scheme (3.20), and  $D_- = \kappa_\alpha D_+$  and  $E_- = \kappa_\beta E_+$ , then there is a positive constant  $C$  such that

$$\|u(x_i, y_j, t_n) - u_{i,j}^n\|_2 \leq C(\tau^2 + (\Delta x)^4 + (\Delta y)^4),$$

with  $i = 1, 2, \dots, N_x - 1; j = 1, 2, \dots, N_y - 1; n = 0, 1, \dots, N_t$ .

*Proof.* Taking  $e_{i,j}^n = u(x_i, y_j, t_n) - u_{i,j}^n$ , and subtracting (3.9) from (3.20), we obtain

$$(I - \mathcal{A}_x)(I - \mathcal{A}_y)\mathbf{e}^{n+1} = (I + \mathcal{A}_x)(I + \mathcal{A}_y)\mathbf{e}^n + \mathbf{R}^{n+1}, \quad (4.6)$$

where  $\mathcal{A}_x$  and  $\mathcal{A}_y$  are given in (3.18), and

$$\begin{aligned} \mathbf{e}^n &= [e_{1,1}^n, e_{2,1}^n, \dots, e_{N_x-1,1}^n, e_{1,2}^n, e_{2,2}^n, \dots, e_{N_x-1,2}^n, \dots, e_{1,N_y-1}^n, e_{2,N_y-1}^n, \dots, e_{N_x-1,N_y-1}^n]^T, \\ \mathbf{R}^n &= [R_{1,1}^n, R_{2,1}^n, \dots, R_{N_x-1,1}^n, R_{1,2}^n, R_{2,2}^n, \dots, R_{N_x-1,2}^n, \dots, R_{1,N_y-1}^n, R_{2,N_y-1}^n, \dots, R_{N_x-1,N_y-1}^n]^T, \end{aligned}$$

and  $|R_{i,j}^{n+1}| \leq \tilde{c}\tau(\tau^2 + (\Delta x)^4 + (\Delta y)^4)$  is given in (3.10).

From (4.4),  $\mathcal{A}_x$  and  $\mathcal{A}_y$  commute, then Eq. (4.6) can be rewritten as

$$\mathbf{e}^{n+1} = (I - \mathcal{A}_x)^{-1} (I + \mathcal{A}_x) (I - \mathcal{A}_y)^{-1} (I + \mathcal{A}_y) \mathbf{e}^n + (I - \mathcal{A}_x)^{-1} (I - \mathcal{A}_y)^{-1} \mathbf{R}^{n+1}.$$

Again, similar to the proof of Theorem 4.2 of [Deng & Chen (2013)], we know that  $\|(I - \mathcal{A}_v)^{-1} (I + \mathcal{A}_v)\|_2$  and  $\|(I - \mathcal{A}_v)^{-1}\|_2$  are less than 1, where  $v = x, y$ . Then there exists

$$\|\mathbf{e}^n\|_2 \leq \sum_{k=0}^{n-1} |\mathbf{R}^{k+1}| \leq c(\tau^2 + (\Delta x)^4 + (\Delta y)^4).$$

$\square$

## 5. Numerical results

In this section, we numerically verify the above theoretical results including convergence rates and numerical stability. And the  $l_\infty$  norm is used to measure the numerical errors.

### 5.1 Numerical results for 1D

Consider the one-dimensional fractional diffusion equation (3.1) in the domain  $0 < x < 2$ ,  $0 < t \leq 1$ , with the variable coefficients  $d_+(x) = x^\alpha$ ,  $d_-(x) = 2x^\alpha$ , and the forcing function

$$f(x,t) = \cos(t+1)x^4(2-x)^4 - x^\alpha \sin(t+1) \left[ \frac{\Gamma(9)}{\Gamma(9-\alpha)}(x^{8-\alpha} + 2(2-x)^{8-\alpha}) - 8 \frac{\Gamma(8)}{\Gamma(8-\alpha)}(x^{7-\alpha} + 2(2-x)^{7-\alpha}) + 24 \frac{\Gamma(7)}{\Gamma(7-\alpha)}(x^{6-\alpha} + 2(2-x)^{6-\alpha}) - 32 \frac{\Gamma(6)}{\Gamma(6-\alpha)}(x^{5-\alpha} + 2(2-x)^{5-\alpha}) + 16 \frac{\Gamma(5)}{\Gamma(5-\alpha)}(x^{4-\alpha} + 2(2-x)^{4-\alpha}) \right],$$

and the initial condition  $u(x,0) = \sin(1)x^4(2-x)^4$ , the boundary conditions  $u(0,t) = u(1,t) = 0$ , and the exact solution of the equation is  $u(x,t) = \sin(t+1)x^4(2-x)^4$ .

Table 1. The maximum errors and convergent orders for the scheme (3.7) of the one-dimensional fractional diffusion equation (3.1) at  $t=1$  and  $\tau = h^2$ .

$(p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s})$	$h$	$\alpha = 1.1$	Rate	$\alpha = 1.9$	Rate
(1,2,1,0,1,2,1,-2)	1/10	4.7842e-03		5.8264e-03	
	1/20	2.5436e-04	4.2333	5.9999e-04	3.2796
	1/40	1.9662e-05	3.6934	4.6242e-05	3.6977
	1/60	4.1748e-06	3.8218	9.7725e-06	3.8334
(1,2,1,-3,1,2,1,-2)	1/10	8.5475e-03		5.5003e-03	
	1/20	4.9722e-04	4.1035	5.7476e-04	3.2585
	1/40	3.9559e-05	3.6518	4.4490e-05	3.6914
	1/60	8.6604e-06	3.7464	9.4148e-06	3.8301

Table 1 shows the maximum errors, at time  $t = 1$  with  $\tau = h^2$ , the numerical results confirm the convergence with the global truncation error  $\mathcal{O}(\tau^2 + h^4)$ .

### 5.2 Numerical results for 2D

Consider the two-dimensional fractional diffusion equation (1.2), where  $0 < x < 2$ ,  $0 < y < 2$ , and  $0 < t \leq 1$ , with the variable coefficients  $d_+(x,y) = x^\alpha$ ,  $d_-(x,y) = 2x^\alpha$ , and  $e_+(x,y) = y^\beta$ ,  $e_-(x,y) = 2y^\beta$ , and the initial condition  $u(x,y,0) = \sin(1)x^4(2-x)^4y^4(2-y)^4$  with the zero boundary conditions, and the exact solution of the equation is

$$u(x,y,t) = \sin(t+1)x^4(2-x)^4y^4(2-y)^4.$$

From the above conditions, it is easy to get the forcing function  $f(x,y,t)$ .

Table 2 displays the maximum errors of the scheme (3.20), and confirms the desired convergence with the global truncation error  $\mathcal{O}(\tau^2 + (\Delta x)^4 + (\Delta y)^4)$ .

## 6. Conclusions

Based on the Lubich's operators, this work provides a new idea to obtain the high order discretization schemes for space fractional derivative. We obtain the effective difference operators with 2nd order,

Table 2. The maximum errors and convergent orders for the scheme (3.20) of the two-dimensional fractional diffusion equation (1.2) at  $t=1$  and  $\tau = (\Delta x)^2 = (\Delta y)^2$ .

$(p, q, r, s, \bar{p}, \bar{q}, \bar{r}, \bar{s})$	$\Delta x$	$\alpha = \beta = 1.1$	Rate	$\alpha = 1.8, \beta = 1.9$	Rate
(1,2,1,0,1,2,1,-2)	1/10	8.6154e-03		6.5211e-03	
	1/20	5.4115e-04	3.9928	4.4802e-04	3.8635
	1/30	1.2626e-04	3.5894	8.8416e-05	4.0023
	1/40	4.3328e-05	3.7177	2.7791e-05	4.0229
(1,2,1,-3,1,2,1,-2)	1/10	1.0110e-02		6.6368e-03	
	1/20	6.3881e-04	3.9842	4.5471e-04	3.8675
	1/30	1.4363e-04	3.6806	8.9704e-05	4.0032
	1/40	4.8431e-05	3.7788	2.8199e-05	4.0226

3rd order, and 4th order accuracy, called WSLD operators. For further checking the efficiency of the high order schemes, we apply the 4th order scheme to solve the space fractional diffusion equation with variable coefficients; and the detailed theoretical analysis and numerical verifications are presented. Hopefully, the higher order (5th order, 6th order, etc.) schemes can be obtained by following the idea given in this paper. In fact, for any fixed convergent order, the obtained difference operators are a class of difference operators, not just one particular operator.

### Acknowledgments

This work was supported by the National Natural Science Foundation of China under Grant No. 11271173 and the Program for New Century Excellent Talents in University under Grant No. NCET-09-0438.

### References

- CHAN, R. H. & JIN, X. Q. (2007) *An Introduction to Iterative Toeplitz Solvers*. SIAM.
- CHEN, M. H. & DENG, W. H. (2011) A second-order numerical method for two-dimensional two-sided space fractional convection diffusion equation. arXiv: 1304.3788 [math.NA].
- CHEN, M. H., DENG, W. H. & WU, Y. J. (2013) Superlinearly convergent algorithms for the two-dimensional space-time Caputo-Riesz fractional diffusion equation. *Appl. Numer. Math.*, **70**, 22–41.
- CHEN, M. H., WANG, Y. T., CHENG, X. & DENG, W. H. (2012) Second-order LOD multigrid method for multidimensional Riesz fractional diffusion equation. arXiv:1301.2643v1 [math.NA].
- CUESTA, E., LUBICH, CH. & PALENCIA, C. (2006) Convolution quadrature time discretization of fractional diffusion-wave equations. *Math. Comput.*, **75**, 673–696.
- DENG, W. H. & CHEN, M. H. (2013) Efficient numerical algorithms for three-dimensional fractional partial differential equations. arXiv:1303.4628v1 [math.NA].
- DIETHELM, K. (2010) *The Analysis of Fractional Differential Equations*. Springer-Verlag Berlin Heidelberg.

- DOUGLS, J. (1955) On the numerical integration of  $u_{xx} + u_{yy} = u_{tt}$  by implicit methods. *J. Soc. Indust. Appl. Math.*, **3**, 42–65.
- ERVIN, V. J. & ROOP, J. P. (2006) Variational formulation for the stationary fractional advection dispersion equation. *Numer. Methods Partial Differential Equations.*, **22**, 558–576.
- HENRICI, P. (1962) *Discrete Variable Methods in Ordinary Differential Equations*. New York: John Wiley.
- LAUB, A. J. (2005) *Matrix Analysis for Scientists and Engineers*. SIAM.
- LUBICH, CH. (1986) Discretized fractional calculus. *SIAM J. Math. Anal.*, **17**, 704–719.
- MEERSCHAERT, M. M. & TADJERAN, C. (2004) Finite difference approximations for fractional advection-dispersion flow equations. *J. Comput. Appl. Math.*, **172**, 65–77.
- PEACEMAN, D. & RACHFORD, H. (1955) The numerical solution of parabolic and elliptic differential equations. *J. Soc. Indust. Appl. Math.*, **3**, 28–41.
- PODLUBNY, I. (1999) *Fractional Differential Equations*. New York: Academic Press.
- QUARTERONI, A., SACCO, R. & SALERI, F. (2007) *Numerical Mathematics, 2nd ed.* Springer.
- SAMKO, S., KILBAS, A. & MARICHEV, O. (1993) *Fractional Integrals and Derivatives: Theory and Applications*. Gordon and Breach, London.
- SOUSA, E. & LI, C. (2011) A weighted finite difference method for the fractional diffusion equation based on the Riemann-Liouville derivative. arXiv:1109.2345v1 [math.NA].
- SUN, Z. Z. & WU, X. N. (2006) A fully discrete difference scheme for a diffusion-wave system. *Appl. Numer. Math.*, **56**, 193–209.
- TIAN, W. Y., ZHOU, H. & DENG, W. H. (2012) A class of second order difference approximations for solving space fractional diffusion Equations. arXiv:1204.4870v1 math.NA.
- YUSTE, S. B. (2006) Weighted average finite difference methods for fractional diffusion equations. *J. Comput. Phys.*, **216**, 264–274.
- ZHUANG, P., LIU, F., ANH, V. & TURNER, I. (2009) Numerical methods for the variable-order fractional advection-diffusion equation with a nonlinear source term. *SIAM J. Numer. Anal.*, **47**, 1760–1781.