Communications in Applied and Industrial Mathematics, ISSN 2038-0909, e-536 DOI: 10.1685/journal.caim.536

High-order approximation to Caputo derivatives and Caputo-type advection-diffusion equations [a]

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Dedicated to Professor Francesco Mainardi on the occasion of his retirement

Communicated by Gianni Pagnini and Enrico Scalas

Abstract

In this paper, a high order approximation with convergence order $O(\tau^{3-\alpha})$ to Caputo derivative ${}_C D_{0,t}^{\alpha} f(t)$ for $\alpha \in (0,1)$ is introduced. Furthermore, two high-order algorithms for Caputo type advection-diffusion equation are obtained. The stability and convergence are rigorously studied which depend upon the derivative order α. The corresponding convergence orders are $O(\tau^{3-\alpha} + h^2)$ and $O(\tau^{3-\alpha} + h^4)$, where τ is the time stepsize, h the space stepsize, respectively. Finally, numerical examples are given to support the theoretical analysis.

Keywords: `Caputo derivative, Fractional advection-diffusion equation, Difference scheme, Stability, Convergence.`

AMS subject classification: `65M06 65M12.`

1. Introduction.

Constructing numerical methods for fractional integrals and fractional derivatives is always one of the central topics in numerical fractional calculus. From the bibliographical references available, among the fractional integrals, the Reimann-Liouville integral is mostly used. And amongst the fractional derivatives, the Riemann-Liouville derivative and the Caputo derivative are often adopted [1–5]. Numerical approaches to Riemann-Liouville

[a]This work was supported by the National Natural Science Foundation of China (grant 11372170), the Key Program of Shanghai Municipal Education Commission (grant 12ZZ084), and the grant The First-class Discipline of Universities in Shanghai.

Received on 01 20, 2014. Accepted on 09 23, 2014. Published on 08 10, 2015.

integral and derivative are mainly derived by using the discrete Grünwald-Letnikov derivative and its various variants [6–8]. Numerical algorithms for Caputo derivative have recently received attention and attracted increasing interests [9–13]. As far as we know, Lubich was the first one who studied the high-order numerical algorithms for Riemann-Liouville integral and Riemann-Liouville derivative [6]. Li, et al., were the early ones who constructed the high-order numerical methods for Caputo derivative, where the convergence order is the second order [12]. In very recent, Gao, et al., considered a high-order algorithm with convergence order $(3-\alpha)$ for Caputo derivative [13]. We admit their priority of $(3-\alpha)$th order scheme for Caputo derivative. In this paper, we also introduce a $(3-\alpha)$ order algorithm for Caputo derive with a slightly different method, where the expressions of weight coefficients presented are very easily analyzed. The important properties of these coefficients are firstly studied which are conveniently applied to unconditional stability analysis and convergence analysis.

Next, we study the standard time fractional advection-diffusion equation in the following form,

$$\begin{cases} {}_CD_{0,t}^{\alpha}u(x,t) = K_{\alpha}\dfrac{\partial^2 u(x,t)}{\partial x^2} \\ \qquad\qquad - V_{\alpha}\dfrac{\partial u(x,t)}{\partial x} + f(x,t),\ 0<x<L,\ t>0, \\ u(x,0)=\phi(x),\ 0\le x\le L, \\ u(0,t)=\varphi(t),\ u(L,t)=\psi(t),\ t>0, \end{cases} \tag{1}$$

where $K_{\alpha}>0$ is the diffusion coefficient, $V_{\alpha}>0$ the advection coefficient, and ${}_CD_{0,t}^{\alpha}$ denotes the Caputo derivative operator with order $\alpha\in(0,1)$, defined by

$${}_CD_{0,t}^{\alpha}f(t)=\frac{1}{\Gamma(1-\alpha)}\int_0^t (t-s)^{-\alpha}f'(s)ds,$$

in which $\Gamma(\cdot)$ is the Euler Gamma function. The somewhat special forms of the above equation were studied in [14–17].

The outline of this paper is organized as follows. In Section 2, a much higher order algorithm for Caputo derivative ${}_CD_{0,t}^{\alpha}f(t)$ with order $\alpha\in(0,1)$ is detailedly constructed. The weight coefficients in the numerical scheme for this derivative are studied. Based on the derived scheme, two numerical methods for equation (1) are proposed in Sections 3 and 4, where the stability, convergence with order $O(\tau^{3-\alpha}+h^2)$ and $O(\tau^{3-\alpha}+h^4)$ are rigorously studied, in which τ is the temporal steplength, and h the spatial one. In Section 5, we give some numerical examples to support the derived theoretical results. The last section concludes this article.

2. Numerical approach to Caputo derivative

In recent, Gao et al. presented a $(3-\alpha)$th order algorithm for Caputo derivative and applied it to numerical computations of fractional partial differential equations, where the stability and convergence analysis, and error estimates, have not been derived yet [13]. In this paper, we use a slightly different method to derive a $(3-\alpha)$th order scheme for Caputo ${}_CD^{\alpha}_{0,t}f(t)$ with $\alpha \in (0,1)$. Especially, the important properties of the weight coefficients in the established numerical scheme are studied which are very useful for stability analysis and convergence analysis.

Suppose that $f^{(5)}(t)$ is continuous and $f^{(6)}(t)$ exists on the interval $[0,T]$. Let $0 = t_0 < t_1 < ... < t_N = T$, and $t_k = k\tau$, in which $\tau = \frac{T}{N}$, $k = 0, 1, ..., N$. Firstly, using the Taylor expansion to $f'(s), f(t_{i-1}), f(t_{i+1})$ at the point $t = t_i$ $(0 \leq i < k)$, one gets

$$\begin{aligned} f'(s) &= f'(t_i) + f''(t_i)(s-t_i) \\ &\quad + \frac{f^{(3)}(t_i)}{2!}(s-t_i)^2 + O((s-t_i)^3), \;\; s \in (t_i, t_{i+1}), \\ f'(t_i) &= \frac{f(t_{i+1}) - f(t_{i-1})}{2\tau} - \frac{f^{(3)}(t_i)}{3!}\tau^2 + O(\tau^4), \end{aligned}$$

and,

$$f''(t_i) = \frac{f(t_{i+1}) - 2f(t_i) + f(t_{i-1})}{\tau^2} - \frac{f^{(4)}(t_i)}{12}\tau^2 + O(\tau^4).$$

Hence we can obtain that

$$\begin{aligned} f'(s) &= \frac{f(t_{i+1}) - f(t_{i-1})}{2\tau} + \frac{f(t_{i+1}) - 2f(t_i) + f(t_{i-1})}{\tau^2}(s-t_i) \\ &\quad - \frac{f^{(3)}(t_i)}{3!}\tau^2 + \frac{f^{(3)}(t_i)}{2!}(s-t_i)^2 + O((s-t_i)^3), \\ &\quad 0 < s - t_i < \tau. \end{aligned} \tag{2}$$

So the Caputo derivative can be discretized as

$$
\begin{aligned}
{}_C D_{0,t}^{\alpha} f(t)\Big|_{t=t_k} &= \frac{1}{\Gamma(1-\alpha)} \int_0^{t_k} (t_k - s)^{-\alpha} f'(s) ds \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{i=0}^{k-1} \int_{t_i}^{t_{i+1}} (t_k - s)^{-\alpha} f'(s) ds \\
&= \frac{1}{\Gamma(1-\alpha)} \sum_{i=0}^{k-1} \int_{t_i}^{t_{i+1}} (t_k - s)^{-\alpha} \Big[\frac{f(t_{i+1}) - f(t_{i-1})}{2\tau} \\
&+ \frac{f(t_{i+1}) - 2f(t_i) + f(t_{i-1})}{\tau^2} \cdot (s - t_i) \\
&- \frac{f^{(3)}(t_i)}{3!}\tau^2 + \frac{f^{(3)}(t_i)}{2!}(s - t_i)^2 \Big] ds + O(\tau^3) \\
&= \frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} [w_{1,k-i}(f_{i+1} - f_{i-1}) \\
&+ w_{2,k-i}(f_{i+1} - 2f_i + f_{i-1})] + r^k,
\end{aligned} \tag{3}
$$

where $f_{i+1} = f(t_{i+1}), f_i = f(t_i)$, and $f_{i-1} = f(t_{i-1})$,

$$w_{1,k-i} = \frac{2-\alpha}{2}\big[(k-i)^{1-\alpha} - (k-i-1)^{1-\alpha}\big], \tag{4}$$

$$w_{2,k-i} = (k-i)^{2-\alpha} - (k-i-1)^{2-\alpha} - (2-\alpha)(k-i-1)^{1-\alpha}, \tag{5}$$

$i = 0, 1, ..., k-1,\ k = 1, 2, ..., N$, and r^k is the truncation error in the following form,

$$r^k = \frac{1}{\Gamma(1-\alpha)} \sum_{i=0}^{k-1} \int_{t_i}^{t_{i+1}} (t_k - s)^{-\alpha} \big[-C_f\tau^2 + 3C_f(s-t_i)^2 \big] ds + O(\tau^3), \tag{6}$$

in which $C_f = \frac{f^{(3)}(t_i)}{3!}$ is a constant depending only upon f.

For the right-hand side of equation (6), we have

$$\frac{1}{\Gamma(1-\alpha)} \sum_{i=0}^{k-1} \int_{t_i}^{t_{i+1}} (t_k - s)^{-\alpha} \big[-C_f\tau^2 + 3C_f(s-t_i)^2 \big] ds = \frac{C_f}{\Gamma(1-\alpha)} \sum_{i=0}^{k-1} (I_1 + 3I_2),$$

DOI: 10.1685/journal.caim.536

in which

$$
\begin{aligned}
I_1 &= -\int_{t_i}^{t_{i+1}} (t_k - s)^{-\alpha}\tau^2 ds = \frac{\tau^{3-\alpha}}{1-\alpha}[(k-i-1)^{1-\alpha} - (k-i)^{1-\alpha}],\\
I_2 &= \int_{t_i}^{t_{i+1}} (t_k - s)^{-\alpha}(s-t_i)^2 ds\\
&= -\frac{\tau^{3-\alpha}}{1-\alpha}(k-i-1)^{1-\alpha} - \frac{2\tau^{3-\alpha}}{(1-\alpha)(2-\alpha)}(k-i-1)^{2-\alpha}\\
&\quad - \frac{2\tau^{3-\alpha}}{(1-\alpha)(2-\alpha)(3-\alpha)}\big[(k-i-1)^{3-\alpha} - (k-i)^{3-\alpha}\big].
\end{aligned}
$$

Therefore,

$$
\begin{aligned}
\frac{C_f}{\Gamma(1-\alpha)}\sum_{i=0}^{k-1}(I_1+3I_2) =& \frac{C_f\tau^{3-\alpha}}{\Gamma(2-\alpha)}\Big\{ -k^{1-\alpha} - 3\big[(k-1)^{1-\alpha} + ... + 2^{1-\alpha} + 1\big]\\
&- \frac{6}{2-\alpha}\big[(k-1)^{2-\alpha} + ... + 2^{2-\alpha} + 1\big] + \frac{6}{(2-\alpha)(3-\alpha)}k^{3-\alpha}\Big\}.
\end{aligned}
$$

Let

$$
\begin{aligned}
S(k) =& -3\sum_{i=1}^{k-1} i^{1-\alpha} - \frac{6}{2-\alpha}\sum_{i=1}^{k-1} i^{2-\alpha} + \frac{6}{(2-\alpha)(3-\alpha)}k^{3-\alpha} - k^{1-\alpha}\\
&\triangleq \sum_{i=0}^{k-1} a_i,\ k \geq 1.
\end{aligned}
\tag{7}
$$

If $k = 1$, define $a_0 = s(1) = \dfrac{6}{(2-\alpha)(3-\alpha)} - 1$. Then a_i $(i \geq 1)$ can be defined as follows,

$$
a_i = S(i+1) - S(i) = \frac{6}{(2-\alpha)(3-\alpha)}[(i+1)^{3-\alpha} - i^{3-\alpha}] - \frac{6}{2-\alpha}i^{2-\alpha} - (i+1)^{1-\alpha} - 2i^{1-\alpha}.
$$

Next we show that $|S(k)|$ is bounded for $k \geq 1$. This leads us to prove the series $\sum_{i=0}^{\infty} a_i$ converges.

In fact, for $i \geq 2$,

$$\begin{aligned}
\big|a_i\big| =& i^{2-\alpha}\Big|\frac{6i}{(2-\alpha)(3-\alpha)}\Big[(1+\frac{1}{i})^{3-\alpha}-1\Big]-\frac{6}{2-\alpha}-\frac{1}{i}(1+\frac{1}{i})^{1-\alpha}-\frac{2}{i}\Big| \\
=& i^{2-\alpha}\Big|\frac{6i}{(2-\alpha)(3-\alpha)}\Big[-1+1+(3-\alpha)\frac{1}{i}+\frac{(3-\alpha)(2-\alpha)}{2!}\frac{1}{i^2} \\
&+\frac{(3-\alpha)(2-\alpha)(1-\alpha)}{3!}\frac{1}{i^3}+\frac{(3-\alpha)(2-\alpha)(1-\alpha)(-\alpha)}{4!}\frac{1}{i^4} \\
&+\frac{(3-\alpha)(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)}{5!}\frac{1}{i^5} \\
&+\frac{(3-\alpha)(2-\alpha)(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)}{6!}\frac{1}{i^6}+...\Big] \\
&-\frac{6}{2-\alpha}-\frac{1}{i}\Big[1+(1-\alpha)\frac{1}{i}+\frac{(1-\alpha)(-\alpha)}{2!}\frac{1}{i^2}+\frac{(1-\alpha)(-\alpha)(-\alpha-1)}{3!}\frac{1}{i^3} \\
&+\frac{(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)}{4!}\frac{1}{i^4}+...\Big]-\frac{2}{i}\Big| \\
=& i^{2-\alpha}\Big|(\frac{6}{4!}-\frac{1}{2!})(1-\alpha)(-\alpha)\frac{1}{i^3}+(\frac{6}{5!}-\frac{1}{3!})(1-\alpha)(-\alpha)(-\alpha-1)\frac{1}{i^4} \\
&+(\frac{6}{6!}-\frac{1}{4!})(1-\alpha)(-\alpha)(-\alpha-1)(-\alpha-2)\frac{1}{i^5}+...\Big| \\
\leq& \frac{1}{4}i^{2-\alpha}(1-\alpha)\alpha\frac{1}{i^3}\Big[1+\frac{7}{15}(1+\alpha)\frac{1}{i}+\frac{2}{15}(1+\alpha)(2+\alpha)\frac{1}{i^2} \\
&+\frac{1}{35}(1+\alpha)(2+\alpha)(3+\alpha)\frac{1}{i^3}+\frac{1}{504}(1+\alpha)(2+\alpha)(3+\alpha)(4+\alpha)\frac{1}{i^4}+...\Big] \\
\leq& \frac{1}{4}(1-\alpha)\alpha\frac{1}{i^{1+\alpha}}(1+\frac{1}{i}+\frac{1}{i^2}+...) \\
\leq& \frac{1}{4}(1-\alpha)\alpha\frac{1}{i^{1+\alpha}}\frac{1}{1-\frac{1}{i}}\leq\frac{2}{4}(1-\alpha)\alpha\frac{1}{i^{1+\alpha}}\leq\frac{1}{8}\frac{1}{i^{1+\alpha}}.
\end{aligned}$$

So series $\sum_{i=2}^{\infty} a_i$ converges, which means that $S(k)$ is bounded by a constant C_1. Therefore,

$$\Big|\frac{C_f}{\Gamma(1-\alpha)}\sum_{i=0}^{k-1}(I_1+3I_2)\Big|=\frac{C_f\tau^{3-\alpha}}{\Gamma(2-\alpha)}|S(k)|\leq\frac{C_fC_1}{\Gamma(2-\alpha)}\tau^{3-\alpha}.$$

It immediately follows that

$$r^k \leq C\tau^{3-\alpha}. \tag{8}$$

DOI: 10.1685/journal.caim.536

So the Caputo derivative has the following numerical approximation,
(9)

$$\begin{aligned} {}_C D_{0,t_k}^{\alpha} f(t_k) = & \frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} \left[w_{1,k-i}(f_{i+1} - f_{i-1}) + w_{2,k-i}(f_{i+1} - 2f_i + f_{i-1}) \right] \\ & + O(\tau^{3-\alpha}),\ k = 1,2,...,N,\ t_k = k\tau \le N\tau = T, \end{aligned}$$

where $0 < \alpha < 1$, $w_{1,k-i}$ and $w_{2,k-i}$ are defined by (4) and (5).

Remark 2.1. In formula (9), if $i = 0$, then $f_{i-1} = f_{-1}$ is defined outside of $[0, T]$. Here, we give various choices to approach f_{-1}. In numerical calculation, we mainly use the neighbouring function values to approximate f_{-1}, that is, $f_{-1} = f(0) - \tau f'(0) + \frac{\tau^2}{2} f''(0) + O(\tau^3)$.
1) When $f'(0) = f''(0) = 0$, then $f_{-1} = f_0 + O(\tau^3)$, the convergence order of (9) is $O(\tau^{3-\alpha})$.
2) When $f'(0) = 0,\ f''(0) \neq 0$, then $f_{-1} = f_0 + \frac{\tau^2}{2} f''(0) + O(\tau^3)$, the convergence order of (9) is $O(\tau^2)$.
3) When $f'(0) \neq 0$, then the convergence order is $O(\tau)$.

In the following, we focus on studying the properties of the weight coefficients $w_{1,k-i}$ and $w_{2,k-i}$.

Lemma 2.1. *The coefficients $w_{1,k-i}$ and $w_{2,k-i}$ $(k = 1, 2, ..., N,\ i = 0, 1, ..., k-1)$ defined by (4) and (5) for $\alpha \in (0, 1)$ satisfy the following properties*

(I) $w_{1,1} = \dfrac{2-\alpha}{2},\ w_{2,1} = 1;$

(II) $0 < w_{1,k-i+1} < w_{1,k-i} \le \dfrac{2-\alpha}{2} < 1, 0 < w_{2,k-i+1} < w_{2,k-i} \le 1;$

(III) $w_{1,k-i+1} - w_{1,k-i} > w_{1,k-i} - w_{1,k-i-1},\ k - i \ge 2;$

$w_{2,k-i+1} - w_{2,k-i} > w_{2,k-i} - w_{2,k-i-1},\ k - i \ge 2;$

(IV) $w_{1,2} + w_{1,1} + w_{2,2} - w_{2,1} \begin{cases} > 0, & \text{if } \alpha \in (0, \alpha_0), \\ \le 0, & \text{if } \alpha \in [\alpha_0, 1), \end{cases}$

where $\alpha_0 \approx 0.68$ is the unique zero point of $(6-\alpha)2^{-\alpha} + \alpha - 4 = 0$ for $\alpha \in (0, 1)$;

$w_{1,k-i} + w_{1,k-i-1} + w_{2,k-i} - w_{2,k-i-1} > 0,\ \ k-i \geq 3;$

$(V)\ \ -w_{1,2} + 2w_{2,1} - w_{2,2} > 0;$

$$w_{1,3} - w_{1,1} + w_{2,3} - 2w_{2,2} + w_{2,1} \begin{cases} < 0, \ \text{if } \alpha \in (0, \alpha_1), \\ \geq 0, \ \text{if } \alpha \in [\alpha_1, 1), \end{cases}$$

where $\alpha_1 \approx 0.37$ is the unique zero point of

$$-2^{3-\alpha} + 3^{2-\alpha} - 2^{2-\alpha} + \frac{2-\alpha}{2}3^{1-\alpha} - \frac{3(2-\alpha)}{2}2^{1-\alpha} - \frac{3\alpha}{2} + 6 = 0 \text{ for } \alpha \in (0,1);$$

$w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1} < 0, k-i \geq 3.$

Proof. (I) It is obvious from the definitions of $w_{1,k-i}$ and $w_{2,k-i}$.
(II) Let $j = k - i$, then (4) and (5) can be rewritten as

$$\begin{aligned} w_{1,j} &= \frac{2-\alpha}{2}[j^{1-\alpha} - (j-1)^{1-\alpha}], \\ w_{2,j} &= j^{2-\alpha} - (j-1)^{2-\alpha} - (2-\alpha)(j-1)^{1-\alpha}. \end{aligned}$$

Suppose

$$\begin{aligned} f_1(x) &= x^{1-\alpha} - (x-1)^{1-\alpha}, \\ f_2(x) &= x^{2-\alpha} - (x-1)^{2-\alpha} - (2-\alpha)(x-1)^{1-\alpha}, \end{aligned}$$

where $x > 1$. Noticing that $0 < \alpha < 1$, one has

$$f_1'(x) = (1-\alpha)[x^{-\alpha} - (x-1)^{-\alpha}] < 0, \ x > 1,$$

so $f_1(j+1) < f_1(j)$, i.e., $w_{1,j+1} < w_{1,j}$.

$$\begin{aligned} f_2'(x) &= (2-\alpha)[x^{1-\alpha} - (x-1)^{1-\alpha} - (1-\alpha)(x-1)^{-\alpha}] \\ &= (2-\alpha)(1-\alpha)[\xi^{-\alpha} - (x-1)^{-\alpha}] < 0, \ \xi \in (x-1, x), \end{aligned}$$

so $w_{2,j+1} < w_{2,j}$.
(III) Simple calculations give

$$w_{1,j+1} - w_{1,j} = \frac{2-\alpha}{2}[(j+1)^{1-\alpha} - 2j^{1-\alpha} + (j-1)^{1-\alpha}].$$

Let $g(x) = (x+1)^{1-\alpha} - 2x^{1-\alpha} + (x-1)^{1-\alpha}, \ x > 1$, then $g'(x) = (1-\alpha)[(x+1)^{-\alpha} - 2x^{-\alpha} + (x-1)^{-\alpha}]$.

Suppose $h(x) = (x+1)^{-\alpha} - x^{-\alpha}$, then $h'(x) = -\alpha[(x+1)^{-\alpha-1} - x^{-\alpha-1}] > 0$, hence $g'(x) = (1-\alpha)[h(x) - h(x-1)] > 0$, that is, $g(x)$ is a monotonely increasing function. Then $w_{1,j+1} - w_{1,j} = \frac{2-\alpha}{2}g(j)$ monotonically increases, which follows that

$$w_{1,k-i+1} - w_{1,k-i} > w_{1,k-i} - w_{1,k-i-1}.$$

Similarly,

$$w_{2,j+1} - w_{2,j} = (j+1)^{2-\alpha} - j^{2-\alpha} - (2-\alpha)j^{1-\alpha} - j^{2-\alpha} + (j-1)^{2-\alpha} + (2-\alpha)(j-1)^{1-\alpha}.$$

Let

$$p(x) = (x+1)^{2-\alpha} - 2x^{2-\alpha} - (2-\alpha)x^{1-\alpha} + (x-1)^{2-\alpha} + (2-\alpha)(x-1)^{1-\alpha}, \ x > 1.$$

Then

$$p'(x) = (2-\alpha)\{(x+1)^{1-\alpha} - x^{1-\alpha} - (1-\alpha)x^{-\alpha} - [x^{1-\alpha} - (x-1)^{1-\alpha} - (1-\alpha)(x-1)^{-\alpha}]\}.$$

Set $q(x) = (x+1)^{1-\alpha} - x^{1-\alpha} - (1-\alpha)x^{-\alpha}$. It follows that

$$\begin{aligned} q'(x) &= (1-\alpha)[(x+1)^{-\alpha} - x^{-\alpha} + \alpha x^{-\alpha-1}] \\ &= (1-\alpha)(-\alpha\xi^{-\alpha-1} + \alpha x^{-\alpha-1}) \\ &= \alpha(1-\alpha)[x^{-\alpha-1} - \xi^{-\alpha-1}] > 0, \ \xi \in (x-1, x). \end{aligned}$$

Therefore, $p'(x) = (2-\alpha)[q(x) - q(x-1)] > 0$, that is,

$$w_{2,j+1} - w_{2,j} - (w_{2,j} - w_{2,j-1}) = p(j) - p(j-1) > 0.$$

(IV) According to the definitions of $w_{1,k-i}$ and $w_{2,k-i}$, it follows that $w_{1,2} + w_{1,1} + w_{2,2} - w_{2,1} = (6-\alpha)2^{-\alpha} + \alpha - 4$. By theoretical analysis, there exists a unique $\alpha_0 \approx 0.68$, such that $(6-\alpha)2^{-\alpha} + \alpha - 4 = 0$ for $\alpha \in (0,1)$. Next, we show the last inequality of (IV), i.e., $j > 2$. Obviously,

$$\begin{aligned} &w_{1,j} + w_{1,j-1} + w_{2,j} - w_{2,j-1} \\ &= j^{2-\alpha} - 2(j-1)^{2-\alpha} + (j-2)^{2-\alpha} + \frac{2-\alpha}{2}[j^{1-\alpha} - 2(j-1)^{1-\alpha} + (j-2)^{1-\alpha}] \\ &= \{j^{2-\alpha} - (j-1)^{2-\alpha} + \frac{2-\alpha}{2}[j^{1-\alpha} - (j-1)^{1-\alpha}]\} - \{(j-1)^{2-\alpha} - (j-2)^{2-\alpha} \\ &+ \frac{2-\alpha}{2}\big[(j-1)^{1-\alpha} - (j-2)^{1-\alpha}\big]\}. \end{aligned}$$

Assume $g(x) = x^{2-\alpha} - (x-1)^{2-\alpha} + \frac{2-\alpha}{2}[x^{1-\alpha} - (x-1)^{1-\alpha}], \ x > 2$. Then

$$g'(x) = (2-\alpha)[x^{1-\alpha} - (x-1)^{1-\alpha} + \frac{1-\alpha}{2}\big(x^{-\alpha} - (x-1)^{-\alpha}].$$

Let $h(x) = x^{1-\alpha} + \frac{1-\alpha}{2}x^{-\alpha}, \ x > 2$. So,

$$h'(x) = (1-\alpha)(x^{-\alpha} - \alpha\frac{x^{-\alpha-1}}{2}) = (1-\alpha)x^{-\alpha-1}(x - \frac{\alpha}{2}) > 0.$$

Therefore, $g'(x) = (2-\alpha)[h(x) - h(x-1)] > 0$, $g(x) > g(x-1)$, that is,

$$w_{1,j} + w_{1,j-1} + w_{2,j} - w_{2,j-1} = g(x) - g(x-1) > 0.$$

(V) From (I) and (II), one has
$w_{2,1}=1$, $w_{1,2}<1$ and $w_{2,2}<1$, so it is obvious that $-w_{1,2}+2w_{2,1}-w_{2,2}>-1+2-1=0$.
It is easy to get $w_{1,3}-w_{1,1}+w_{2,3}-2w_{2,2}+w_{2,1}=-2^{3-\alpha}+3^{2-\alpha}-2^{2-\alpha}+\frac{2-\alpha}{2}3^{1-\alpha}-\frac{3(2-\alpha)}{2}2^{1-\alpha}-\frac{3\alpha}{2}+6$. By mathematical analysis, there exists a unique $\alpha_1\approx 0.37$, such that $-2^{3-\alpha}+3^{2-\alpha}-2^{2-\alpha}+\frac{2-\alpha}{2}3^{1-\alpha}-\frac{3(2-\alpha)}{2}2^{1-\alpha}-\frac{3\alpha}{2}+6=0$ for $\alpha\in(0,1)$.
Again, one has

$$\begin{aligned}
&w_{1,j+1}-w_{j-1}+w_{2,j+1}-2w_{2,j}+w_{2,j-1}\\
&=\frac{2-\alpha}{2}(j+1)^{1-\alpha}-\frac{3(2-\alpha)}{2}j^{1-\alpha}+\frac{3(2-\alpha)}{2}(j-1)^{1-\alpha}-\frac{2-\alpha}{2}(j-2)^{1-\alpha}\\
&+(j+1)^{2-\alpha}-3j^{2-\alpha}+3(j-1)^{2-\alpha}-(j-2)^{2-\alpha}\\
&=\frac{2-\alpha}{2}\big\{\big[(j+1)^{1-\alpha}-j^{1-\alpha}\big]-2\big[j^{1-\alpha}-(j-1)^{1-\alpha}\big]+\big[(j-1)^{1-\alpha}-(j-2)^{1-\alpha}\big]\big\}\\
&+\big[(j+1)^{2-\alpha}-j^{2-\alpha}\big]-2\big[j^{2-\alpha}-(j-1)^{1-\alpha}\big]+\big[(j-1)^{2-\alpha}-(j-2)^{2-\alpha}\big]\\
&=g(j)-g(j-1),\ j>2,
\end{aligned}$$

where $g(x)=\dfrac{2-\alpha}{2}\big[(x+1)^{1-\alpha}-2x^{1-\alpha}+(x-1)^{1-\alpha}\big]+\big[(x+1)^{2-\alpha}-2x^{2-\alpha}+(x-1)^{2-\alpha}\big]$, $x>2$. By tedious calculations, one gets,

$$\begin{aligned}
g'(x)&=\frac{2-\alpha}{2}(1-\alpha)\big[(x+1)^{-\alpha}-2x^{-\alpha}+(x-1)^{-\alpha}\big]+(2-\alpha)\big[(x-1)^{1-\alpha}\\
&-2x^{1-\alpha}+(x-1)^{1-\alpha}\big]\\
&=(2-\alpha)\big\{\frac{(1-\alpha)}{2}\big[(x+1)^{-\alpha}-x^{-\alpha}\big]+\big[(x+1)^{1-\alpha}-x^{1-\alpha}\big]\\
&-\frac{1-\alpha}{2}\big[x^{-\alpha}-(x-1)^{-\alpha}\big]-\big[x^{1-\alpha}-(x-1)^{1-\alpha}\big]\big\}\\
&=(2-\alpha)\big[h(x)-h(x-1)\big],
\end{aligned}$$

in which $h(x)=\dfrac{(1-\alpha)}{2}\big[(x+1)^{-\alpha}-x^{-\alpha}\big]+\big[(x+1)^{1-\alpha}-x^{1-\alpha}\big],\ x>2$.
Furthermore,

$$\begin{aligned}
h'(x)&=\frac{1-\alpha}{2}(-\alpha)\big[(x+1)^{-\alpha-1}-x^{-\alpha-1}\big]+(1-\alpha)\big[(x+1)^{-\alpha}-x^{-\alpha}\big]\\
&=(1-\alpha)\big\{\big[\frac{-\alpha}{2}(x+1)^{-\alpha-1}+(x+1)^{-\alpha}\big]-\big[\frac{-\alpha}{2}x^{-\alpha-1}+x^{-\alpha}\big]\big\}.
\end{aligned}$$

DOI: 10.1685/journal.caim.536

Last, set $q(x) = \frac{-\alpha}{2}(x+1)^{-\alpha-1} + (x+1)^{-\alpha},\ x > 2$. One has

$$\begin{aligned} q'(x) &= \frac{\alpha(1+\alpha)}{2}(x+1)^{-\alpha-2} - \alpha(x+1)^{-\alpha-1} \\ &= \alpha(x+1)^{-\alpha-2}\big[\frac{1+\alpha}{2} - (x+1)\big] < 0. \end{aligned}$$

It is easy to see $h'(x) < 0$, furthermore, $g'(x) < 0$, which implies

$$w_{1,j+1} - w_{1,j-1} + w_{2,j+1} - 2w_{2,j} + w_{2,j-1} = g(j) - g(j-1) < 0,$$

i.e.,

$$w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1} < 0$$

.

All this completes the proof. □

Remark 2.2. Lemma 2.1 holds for $\alpha \in (0,1)$. If $\alpha = 1$, Lemma 2.1 (IV) and (V) are not true. Here, Lemma 2.1 (IV) and (V) are useful for the following stability analysis.

3. Numerical scheme I

In this section, we use the approximation scheme for Caputo derivative in Section 2 to discretize the time fractional derivative of equation (1). Throughout this paper, we always suppose equation (1) has a unique solution which satisfies $\frac{\partial u(x,0)}{\partial t} = \frac{\partial^2 u(x,0)}{\partial t^2} = 0$ for discussion convenience.

Let $h = \frac{L}{M}$ be the space stepsize with $x_j = jh$, $j = 0, 1, ..., M$. The time interval $[0, T]$, for a given T, is partitioned in Section 2. For the function $u(x,t)$, its exact and approximate solutions at the point (x_j, t_k) are denoted by u_j^k and U_j^k. Let $\mathbf{u}^k = (u_1^k, ..., u_{M-1}^k)^T$ and $\mathbf{U}^k = (U_1^k, ..., U_{M-1}^k)^T$.

In order to derive numerical solution of equ. (1), discretize the first and second-order spatial derivatives by the second-order central difference schemes,

$$\frac{\partial}{\partial x}u(x_j, t_k) = \frac{u_{j+1}^k - u_{j-1}^k}{2h} + O(h^2), \tag{10}$$

$$\frac{\partial^2}{\partial x^2}u(x_j, t_k) = \frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{h^2} + O(h^2). \tag{11}$$

From Section 2, we approximate the time fractional derivative as below,

$$
\begin{aligned}
{}_C D_{0,t}^{\alpha} u(x_j, t_k) = &\frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} \big[w_{1,k-i} (u_j^{i+1} - u_j^{i-1}) \\
&+ w_{2,k-i} (u_j^{i+1} - 2u_j^i + u_j^{i-1}) \big] \\
&+ O(\tau^{3-\alpha}).
\end{aligned} \tag{12}
$$

So the fractional advection-diffusion equation is discretized as follows,

$$
\begin{aligned}
&\frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} \Big[w_{1,k-i} (U_j^{i+1} - U_j^{i-1}) + w_{2,k-i} (U_j^{i+1} - 2U_j^i + U_j^{i-1}) \Big] \\
&= K_\alpha \frac{U_{j+1}^k - 2U_j^k + U_{j-1}^k}{h^2} - V_\alpha \frac{U_{j+1}^k - U_{j-1}^k}{2h} + f_j^k, \\
&1 \le k \le N, \ 1 \le j \le M-1.
\end{aligned} \tag{13}
$$

The initial and boundary conditions of (1) can be rewritten as

$$
\begin{aligned}
&U_j^0 = \phi(x_j), \ j = 0, 1, ..., M-1, \\
&U_0^k = \varphi(t_k), U_M^k = \psi(t_k), \ k = 0, 1, ..., N.
\end{aligned}
$$

Multiplying h^2 in both sides of (13) and introducing the parameter $\mu = \frac{h^2 \tau^{-\alpha}}{\Gamma(3-\alpha)}$ give

$$
\left\{
\begin{aligned}
&\left(-K_\alpha - \frac{V_\alpha h}{2} \right) U_{j-1}^1 + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha) U_j^1 \\
&+ \left(-K_\alpha + \frac{V_\alpha h}{2} \right) U_{j+1}^1 = 2\mu w_{2,1} U_j^0 + \mu (w_{1,1} - w_{2,1}) U_j^{-1} + h^2 f_j^1, \ k = 1, \\
&\left(-K_\alpha - \frac{V_\alpha h}{2} \right) U_{j-1}^k + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha) U_j^k \\
&+ \left(-K_\alpha + \frac{V_\alpha h}{2} \right) U_{j+1}^k \\
&= \mu (-w_{1,2} + 2w_{2,1} - w_{2,2}) U_j^{k-1} \\
&- \mu \sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1}) U_j^i \\
&+ \mu (w_{1,k-1} + 2w_{2,k} - w_{2,k-1}) U_j^0 \\
&+ \mu (w_{1,k} - w_{2,k}) U_j^{-1} + h^2 f_j^k, \ 2 \le k \le N.
\end{aligned}
\right. \tag{14}
$$

DOI: 10.1685/journal.caim.536

According to Remark 2.1, U_j^{-1} can be replaced by the following equation

$$U_j^{-1} = U_j^0 - \tau \frac{\partial U_j^0}{\partial t} + \frac{\tau^2}{2} \frac{\partial^2 U_j^0}{\partial t^2} + O(\tau^3).$$

Moreover, we have supposed $\frac{\partial u(x,0)}{\partial t} = \frac{\partial^2 u(x,0)}{\partial t^2} = 0$, so set $U_j^{-1} = U_j^0$. We can give the following compact form

(15)

$$\begin{cases} \mathbf{A}\mathbf{U}^1 = \mu(w_{1,1} + w_{2,1})\mathbf{U}^0 + h^2\mathbf{F}_1 + \mathbf{H}_1, \ k = 1, \\ \mathbf{A}\mathbf{U}^k = \mu(-w_{1,2} + 2w_{2,1} - w_{2,2})\mathbf{U}^{k-1} - \mu \sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} \\ \qquad + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})\mathbf{U}^i + \mu(w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})\mathbf{U}^0 \\ \qquad + h^2\mathbf{F}_k + \mathbf{H}_k, \ 2 \le k \le N, \end{cases}$$

where the matrix and vector in (15) are defined as follows,

(16)

$$\mathbf{A} = \text{tri}\left[-K_\alpha - \frac{V_\alpha h}{2}, \mu w_{1,1} + \mu w_{2,1} + 2K_\alpha, -K_\alpha + \frac{V_\alpha h}{2}\right], \ 1 \le k \le N,$$

(17)

$$\mathbf{F}_k = \left(f_1^k, f_2^k, ..., f_{M-1}^k\right)^T, \ \ \mathbf{H}_k = \left((K_\alpha + \frac{V_\alpha h}{2})U_0^k, ..., (K_\alpha - \frac{V_\alpha h}{2})U_M^k\right)^T,$$

$1 \le k \le N.$

Theorem 3.1. *The difference system (14) or (15) has an unique solution.*

Proof. In view of [16], we easily known that the eigenvalues of the matrix $\mathbf{A}$ is

$$\lambda_i = 2K_\alpha + \mu(w_{1,1} + w_{2,1}) + 2\sqrt{K_\alpha^2 - \frac{1}{4}V_\alpha^2 h^2}\, \cos\left(\frac{i}{M}\pi\right), \ i = 1, 2, \dots, M-1.$$

Note that $w_{1,1} = \frac{2-\alpha}{2}, w_{2,1} = 1$, and $\mu = \frac{h^2\tau^{-\alpha}}{\Gamma(3-\alpha)} > 0$. Then,

(i) when $K_\alpha^2 - \frac{1}{4}V_\alpha^2 h^2 \ge 0$, one gets

$$\lambda_i > \frac{4-\alpha}{2}\mu > 0;$$

(ii) when $K_\alpha^2 - \frac{1}{4}V_\alpha^2 h^2 < 0$, one has

$$\lambda_i = 2K_\alpha + \frac{4-\alpha}{2}\mu + 2b\cos\left(\frac{i}{M}\pi\right) \imath \ne 0,$$

where $b^2 = -\left(K_\alpha^2 - \frac{1}{4}V_\alpha^2 h^2\right)$, $\imath^2 = -1$.

So $\det(\mathbf{A}) \neq 0$, which indicates that the solution to (14) or (15) exists and is unique. □

In the following, the stability and convergence are studied.

Theorem 3.2. *The local truncation error of scheme (14) is* $O(\tau^{3-\alpha} + h^2)$.

Proof. According to equations (10)-(12), we define the local truncation error R_j^k of difference scheme (14) as follows.

(18)

$$\begin{aligned} R_j^k =& \frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} \left[w_{1,k-i}(u_j^{i+1} - u_j^{i-1}) + w_{2,k-i}(u_j^{i+1} - 2u_j^i + u_j^{i-1})\right] \\ & - K_\alpha \frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{h^2} + V_\alpha \frac{u_{j+1}^k - u_{j-1}^k}{2h} - f_j^k \\ =& \frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} \left[w_{1,k-i}(u_j^{i+1} - u_j^{i-1}) + w_{2,k-i}(u_j^{i+1} - 2u_j^i + u_j^{i-1})\right] \\ & - {}_C D_{0,t}^\alpha u(x_j, t_k) - K_\alpha \left[\frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{h^2} - \frac{\partial^2}{\partial x^2} u(x_j, t_k)\right] \\ & + V_\alpha \left[\frac{u_{j+1}^k - u_{j-1}^k}{2h} - \frac{\partial}{\partial x} u(x_j, t_k)\right] \\ =& O(\tau^{3-\alpha}) - K_\alpha O(h^2) + V_\alpha O(h^2) = O(\tau^{3-\alpha} + h^2). \end{aligned}$$ □

Here we use the Fourier method [15] to discuss the stability of scheme (14). Let $\tilde{U}_j^k$ be the approximate solution of (14). Define

$$\rho_j^k = U_j^k - \tilde{U}_j^k,\ 1 \leq j \leq M-1,\ 0 \leq k \leq N,$$

with the corresponding vector

$$\rho^k = (\rho_1^k, \rho_2^k, ..., \rho_{M-1}^k)^T.$$

Then one can easily get:

(19)

$$\begin{cases} \left(-K_\alpha - \dfrac{V_\alpha h}{2}\right)\rho_{j-1}^1 + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha)\,\rho_j^1 + \left(-K_\alpha + \dfrac{V_\alpha h}{2}\right)\rho_{j+1}^1 \\ = \mu(w_{1,1} + w_{2,1})\rho_j^0,\ k = 1, \\ \left(-K_\alpha - \dfrac{V_\alpha h}{2}\right)\rho_{j-1}^k + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha)\,\rho_j^k + \left(-K_\alpha + \dfrac{V_\alpha h}{2}\right)\rho_{j+1}^k \\ = \mu(-w_{1,2} + 2w_{2,1} - w_{2,2})\rho_j^{k-1} - \mu\displaystyle\sum_{i=1}^{k-2}(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} \\ - 2w_{2,k-i} + w_{2,k-i-1})\rho_j^i + \mu(w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})\rho_j^0,\ 2 \le k \le N. \end{cases}$$

Now let the grid function be

$$\rho^k(x) = \begin{cases} \rho_j^k,\ x_j - \dfrac{h}{2} < x < x_j + \dfrac{h}{2},\ j = 1, 2, ..., M-1, \\ 0,\ 0 \le x \le \dfrac{h}{2} \text{ or } L - \dfrac{h}{2} \le x \le L, \end{cases}$$

then $\rho^k(x)$ can be expanded in a Fourier series

$$\rho^k(x) = \sum_{m=-\infty}^{\infty} d_k(m) e^{\imath 2\pi m x/L},\ 1 \le k \le N,$$

in which

$$d_k(m) = \frac{1}{L}\int_0^L \rho^k(x) e^{-\imath 2\pi m x/L} dx,\ \imath^2 = -1.$$

Set

$$\|\rho^k\|_2 = \left(\sum_{j=1}^{M-1} h|\rho_j^k|^2\right)^{\frac{1}{2}} = \left[\int_0^L |\rho^k(x)|^2 dx\right]^{\frac{1}{2}}.$$

According to the Parseval equality

$$\int_o^L |\rho^k(x)|^2 dx = \sum_{m=-\infty}^{\infty} |d_k(m)|^2,$$

one has

$$\|\rho^k\|_2^2 = \sum_{m=-\infty}^{\infty} |d_k(m)|^2. \tag{20}$$

Based on the above analysis, we suppose that the solution of (19) has the following form,

$$\rho_j^k = d_k e^{\imath \sigma j h},$$

where $\sigma = 2\pi m/L$. Substitution in (19) yields

(21)
$$\begin{cases} d_1 = \dfrac{\mu(w_{1,1}+w_{2,1})d_0}{4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}}, \ k=1, \\ d_k = \dfrac{1}{4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}}\big[\mu(-w_{1,2}+2w_{2,1} \\ \quad - w_{2,2})d_{k-1} - \mu\displaystyle\sum_{i=1}^{k-2}(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})d_i \\ \quad + \mu(w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})d_0\big], \ 2 \le k \le N. \end{cases}$$

Lemma 3.1. *For d_k $(1 \le k \le n)$ defined by (21), if $\alpha \in (0, \alpha_1)$, the following inequality*

$$|d_k| \le |d_0| \tag{22}$$

holds for $k = 1, 2, ..., N$.

Proof. Notice

$$\begin{aligned} &|4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}| \\ &= \sqrt{(4K_\alpha \sin^2\frac{\sigma h}{2} + \mu w_{1,1} + \mu w_{2,1})^2 + V_\alpha^2 h^2 \sin^2\sigma h} \\ &\ge \sqrt{(\mu w_{1,1} + \mu w_{2,1})^2} = \mu(w_{1,1}+w_{2,1}), \ 1 \le k \le N. \end{aligned} \tag{23}$$

For $k = 1$, from the above inequality and (21), we have

$$|d_1| \le \frac{\mu(w_{1,1}+w_{2,1})}{|4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}|}|d_0| \le |d_0|.$$

For $k = 2$,

$$\begin{aligned} |d_2| \le &\frac{1}{|4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}|}\big[\mu|-w_{1,2}+2w_{2,1} \\ &-w_{2,2}|\cdot|d_1| + \mu|w_{1,2}+w_{1,1}+w_{2,2}-w_{2,1}|\cdot|d_0|\big]. \end{aligned}$$

From Lemma 2.1, if $\alpha \in (0, \alpha_0)$, then

$$|d_2| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} [\mu(-w_{1,2} + 2w_{2,1} - w_{2,2})|d_1| + \mu(w_{1,2} + w_{1,1} + w_{2,2} - w_{2,1})|d_0|]$$
$$\leq \frac{\mu(w_{1,1} + w_{2,1})}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} |d_0| \leq |d_0|.$$

Suppose that $|d_n| \leq |d_0|$ holds for $1 \leq n \leq k-1$. From (21), it immediately follows that

$$|d_k| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} [\mu| - w_{1,2} + 2w_{2,1} - w_{2,2}| \cdot |d_{k-1}|$$
$$+\mu|w_{1,3} - w_{1,1} + w_{2,3} - 2w_{2,2} + w_{2,1}| \cdot |d_{k-2}|$$
$$+\mu \sum_{i=1}^{k-3} |(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1}| \cdot |d_i|$$
$$+\mu|w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1}| \cdot |d_0|].$$

From Lemma 2.1, if $\alpha \in (0, \alpha_1)$, one has,

$$|d_k| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} [\mu(-w_{1,2} + 2w_{2,1} - w_{2,2})|d_{k-1}|$$
$$-\mu(w_{1,3} - w_{1,1} + w_{2,3} - 2w_{2,2} + w_{2,1})|d_{k-2}|$$
$$-\mu \sum_{i=1}^{k-3} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})|d_i|$$
$$+\mu(w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})|d_0|]$$
$$\leq \frac{\mu(w_{1,1} + w_{2,1})}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} |d_0| \leq |d_0|.$$

Here, it must be mentioned that the above inequality is true for $\alpha \in (0, \alpha_1)$ but not for $\alpha \in (0, \alpha_0)$.

Thus, the proof is complete. □

Theorem 3.3. *If $\alpha \in (0, \alpha_1)$, the difference scheme defined by (14) is unconditionally stable.*

Proof. From (20) and (22), we can write

$$\|\rho^k\|_2^2 = \sum_{m=-\infty}^{\infty} |d_k(m)|^2 \leq \sum_{m=-\infty}^{\infty} |d_0(m)|^2 = \|\rho^0\|_2^2,$$

so we have

$$\|\rho^k\|_2 \leq \|\rho^0\|_2,$$

which means that the scheme is unconditionally stable. □

Remark 3.1. 1) For the fractional derivative order α, unconditional stability exists in a proper sub-interval of $(0,1)$, i.e., $\alpha \in (0,\alpha_1) \subsetneq (0,1)$. This means that α_1 can not attain 1. Such a phenomenon was early observed and pointed out in [7,8].
2) Generally speaking, the higher order discretization is given for the fractional derivative in a given differential equation, the smaller interval with respect to the fractional derivative order is required for unconditional stability. For details, refer to [8] and this paper.

Next we study the convergence order of scheme (14). Define the truncation error

$$e_j^k = u(x_j,t_k) - U_j^k = u_j^k - U_j^k, k=0,1,...,N, j=0,1,...,M,$$

and set

$$e^k = (e_1^k, e_2^k, ..., e_{M-1}^k)^T,\ R^k = (R_1^k, R_2^k, ..., R_{M-1}^k)^T, k=1,2,...,N.$$

From the first equality of (18), and letting $u_j^{-1} = u_j^0$, one obtains

(24)

$$\begin{cases} \left(-K_\alpha - \dfrac{V_\alpha h}{2}\right) u_{j-1}^1 + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha)\, u_j^1 + \left(-K_\alpha + \dfrac{V_\alpha h}{2}\right) u_{j+1}^1 \\ = \mu(w_{1,1}+w_{2,1})u_j^0 + h^2 f_j^1 + h^2 R_j^1,\ k=1, \\ \left(-K_\alpha - \dfrac{V_\alpha h}{2}\right) u_{j-1}^k + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha)\, u_j^k + \left(-K_\alpha + \dfrac{V_\alpha h}{2}\right) u_{j+1}^k \\ = \mu(-w_{1,2}+2w_{2,1}-w_{2,2})u_j^{k-1} - \mu \displaystyle\sum_{i=1}^{k-2}(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} \\ - 2w_{2,k-i} + w_{2,k-i-1})u_j^i + \mu(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})u_j^0 + h^2 f_j^k + h^2 R_j^k, \\ \quad 2 \leq k \leq N. \end{cases}$$

Subtracting the above equations from equation (14) leads to
(25)

$$\begin{cases} \left(-K_\alpha - \dfrac{V_\alpha h}{2}\right) e_{j-1}^1 + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha)\, e_j^1 + \left(-K_\alpha + \dfrac{V_\alpha h}{2}\right) e_{j+1}^1 \\ = \mu(w_{1,1} + w_{2,1}) e_j^0 + h^2 R_j^1, k = 1, \\ \left(-K_\alpha - \dfrac{V_\alpha h}{2}\right) e_{j-1}^k + (\mu w_{1,1} + \mu w_{2,1} + 2K_\alpha)\, e_j^k + \left(-K_\alpha + \dfrac{V_\alpha h}{2}\right) e_{j+1}^k \\ = \mu(-w_{1,2} + 2w_{2,1} - w_{2,2}) e_j^{k-1} - \mu \displaystyle\sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} \\ - 2w_{2,k-i} + w_{2,k-i-1}) e_j^i + \mu(w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1}) e_j^0 + h^2 R_j^k, \\ \quad 2 \le k \le N, \end{cases}$$

with

$$e_0^k = e_M^k = 0,\ k = 1, 2, ..., N-1,$$
$$e_j^0 = 0,\ j = 1, 2, ..., M-1.$$

Let the grid function be

$$e^k(x) = \begin{cases} e_j^k,\ x_j - \dfrac{h}{2} < x < x_j + \dfrac{h}{2},\ j = 1, 2, ..., M-1, \\ 0,\ 0 \le x \le \dfrac{h}{2},\ \text{or } L - \dfrac{h}{2} \le x \le L, \end{cases}$$

and

$$R^k(x) = \begin{cases} R_j^k,\ x_j - \dfrac{h}{2} < x < x_j + \dfrac{h}{2},\ j = 1, 2, ..., M-1, \\ 0,\ 0 \le x \le \dfrac{h}{2},\ \text{or } L - \dfrac{h}{2} \le x \le L, \end{cases}$$

respectively. Assume that $e^k(x)$ and $R^k(x)$ have the following Fourier series expansions,

$$e^k(x) = \sum_{m=-\infty}^{\infty} \xi_k(m) e^{\imath 2\pi m x/L},\ R^k(x) = \sum_{m=-\infty}^{\infty} \eta_k(m) e^{\imath 2\pi m x/L},\ \imath^2 = -1,$$

where

$$\xi_k(m) = \frac{1}{L} \int_0^L e^k(x) e^{-\imath 2\pi m x/L} dx,\ \eta_k(m) = \frac{1}{L} \int_0^L R^k(x) e^{-\imath 2\pi m x/L} dx.$$

Define

$$\|e^k(x)\|_2^2 = \sum_{j=1}^{M-1} h |e_j^k|^2 = \sum_{m=-\infty}^{\infty} |\xi_k(m)|^2, \tag{26}$$

$$\|R^k(x)\|_2^2 = \sum_{j=1}^{M-1} h|R_j^k|^2 = \sum_{m=-\infty}^{\infty} |\eta_k(m)|^2. \tag{27}$$

Based on the above analysis, we also suppose that

$$e_j^k = \xi_k e^{\imath\sigma jh},\ R_j^k = \eta_k e^{\imath\sigma jh},$$

where $\sigma = 2\pi m/L$. Taking the above expressions into (25) gives

(28)

$$\begin{cases} \xi_1 = \dfrac{h^2\eta_1}{4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}},\ k=1, \\ \xi_k = \dfrac{1}{4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h \sin\sigma h + \mu w_{1,1} + \mu w_{2,1}}\big[\mu(-w_{1,2} + 2w_{2,1} \\ \quad - w_{2,2})\xi_{k-1} - \mu\displaystyle\sum_{i=1}^{k-2}(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} \\ \quad + w_{2,k-i-1})\xi_i + h^2\eta_k\big],\ 2 \le k \le N. \end{cases}$$

Lemma 3.2. *For ξ_k $(k = 1, 2, ..., N)$ defined by (28), if $\alpha \in (0, \alpha_1)$, there exists a positive constant C_2 such that*

$$|\xi_k| \le C_2(1+\tau)^k|\eta_1|, k = 1, 2, ..., N.$$

Proof. From (18) and the left-hand side of (27), one gets

$$\|R^k\|_2 \le C_1\sqrt{L}(\tau^{3-\alpha} + h^2), k = 1, 2, ..., N. \tag{29}$$

Again, based on the convergence of the series in the right-hand side of (27), then there is a positive constant C_2 such that [14]

$$|\eta_k| \equiv |\eta_k(m)| \le C_2\tau|\eta_1| \equiv C_2\tau|\eta_1(m)|, k = 1, 2, ..., N. \tag{30}$$

From (23), for small enough τ, the following inequality holds

$$\begin{aligned} &\left|4K_\alpha \sin^2\frac{\sigma h}{2} + \imath V_\alpha h\sin\sigma h + \mu w_{1,1} + \mu w_{2,1}\right| \ge \mu(w_{1,1} + w_{2,1}) \\ &= \frac{h^2\tau^{-\alpha}}{\Gamma(3-\alpha)}\left(2 - \frac{\alpha}{2}\right) \ge h^2,\ k = 1, 2, ..., N. \end{aligned} \tag{31}$$

When $k = 1$, from the above inequality and (30), the first equation of (28) yields

$$|\xi_1| \le |\eta_1| \le C_2\tau|\eta_1| \le C_2(1+\tau)|\eta_1|. \tag{32}$$

When $k = 2$,

$$|\xi_2| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big[\mu| - w_{1,2} + 2w_{2,1} - w_{2,2}| \cdot |\xi_1| + h^2 |\eta_2|\Big]$$
$$= \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big[\mu|(w_{1,1} + w_{2,1})$$
$$-(w_{1,2} + w_{1,1} + w_{2,2} - w_{2,1})| \cdot |\xi_1| + h^2 |\eta_2|\Big].$$

From Lemma 2.1, if $\alpha \in (0, \alpha_0)$, one has

$$|\xi_2| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big[\mu|w_{1,1} + w_{2,1}| \cdot |\xi_1| + h^2 |\eta_2|\Big]$$
$$\leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big[\mu(w_{1,1} + w_{2,1}) C_2 (1+\tau)|\eta_1| + h^2 C_2 \tau |\eta_1|\Big]$$
$$\leq C_2(1+\tau)|\eta_1| + C_2 \tau |\eta_1| \leq (1+\tau)^2 C_2 |\eta_1|.$$

Suppose that

$$|\xi_n| \leq C_2 (1+\tau)^n |\eta_1|, \quad n = 1, 2, ..., k-1. \tag{33}$$

One can rewrite (28) as

$$|\xi_k| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big[\mu| - w_{1,2} + 2w_{2,1} - w_{2,2}| \cdot |\xi_{k-1}|$$
$$+\mu|(w_{1,3} - w_{1,1} + w_{2,3} - 2w_{2,2} + w_{2,1})| \cdot |\xi_{k-2}|$$
$$+\mu \sum_{i=1}^{k-3} |(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})| \cdot |\xi_i| + h^2 |\eta_k|\Big].$$

From (30), (33) and Lemma 2.1, if $\alpha \in (0, \alpha_1)$, one has

$$|\xi_k| \leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big[\mu(-w_{1,2} + 2w_{2,1} - w_{2,2}) C_2 (1+\tau)^{k-1}$$
$$|\eta_1| - \mu(w_{1,3} - w_{1,1} + w_{2,3} - 2w_{2,2} + w_{2,1}) C_2 (1+\tau)^{k-2} |\eta_1| - \mu \sum_{i=1}^{k-3} (w_{1,k-i+1}$$
$$-w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1}) C_2 (1+\tau)^i |\eta_1| + h^2 C_2 \tau |\eta_1|\Big].$$
$$\leq \frac{1}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} \Big\{(C_2(1+\tau)^{k-1}) \big[\mu(-w_{1,2}$$
$$+2w_{2,1} - w_{2,2}) - \mu(w_{1,3} - w_{1,1} + w_{2,3} - 2w_{2,2} + w_{2,1}) - \mu \sum_{i=1}^{k-3} (w_{1,k-i+1} - w_{1,k-i-1}$$
$$+w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})|\eta_1|\big] + h^2 C_2 \tau |\eta_1|\Big\}$$
$$\leq \frac{C_2(1+\tau)^{k-1} \big[(w_{1,1} + w_{2,1}) - (w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})\big] |\eta_1|}{|4K_\alpha \sin^2 \frac{\sigma h}{2} + \imath V_\alpha h \sin \sigma h + \mu w_{1,1} + \mu w_{2,1}|} + C_2 \tau |\eta_1|$$
$$\leq C_2 (1+\tau)^{k-1} |\eta_1| + C_2 \tau |\eta_1|$$
$$\leq (1+\tau)^k C_2 |\eta_1|.$$

All this ends the proof. □

Next, one has the following error estimate.

Theorem 3.4. *If $\alpha \in (0, \alpha_1)$, the difference scheme (14) is L2-convergent with order $O(\tau^{3-\alpha} + h^2)$.*

Proof. Using Lemma 3.2 and applying (26), (27) and (29), one gets

$$\|e^k\|_2 \leq (1+\tau)^k C_2 \|R^1\|_2 \leq e^{k\tau} C_1 C_2 \sqrt{L}(\tau^{3-\alpha} + h^2).$$

Since $k\tau \leq T$, one has

$$\|e^k\|_2 \leq C(\tau^{3-\alpha} + h^2), \tag{34}$$

in which $C = C_1 C_2 \sqrt{L} e^T$. □

4. Numerical scheme II

In this section, we derive a much higher order scheme as for the space discretization. Let

$$\mathcal{A} = \left(K_\alpha I + \frac{V_\alpha^2 h^2}{12 K_\alpha}\right)\delta_x^2 - V_\alpha \delta_{\overline{x}},\ \mathcal{B} = I + \frac{h^2}{12}\left(\delta_x^2 - \frac{V_\alpha}{K_\alpha}\delta_{\overline{x}}\right),$$

where I is a unit operator, $\delta_{\overline{x}}$ and δ_x^2 are average-central and second central difference operators with respect to x, which are defined by

$$\delta_{\overline{x}} u(x_j, t_k) = \frac{u_{j+1}^k - u_{j-1}^k}{2h},\ \delta_x^2 u(x_j, t_k) = \frac{u_{j+1}^k - 2u_j^k + u_{j-1}^k}{h^2}.$$

Considering the following differential equation

$$K_\alpha \frac{\partial^2 u(x,t)}{\partial x^2} - V_\alpha \frac{\partial u(x,t)}{\partial x} = g(x,t), \tag{35}$$

and referring to [14,17], we obtain a fourth-order difference scheme for solving the equation (1) as follows

$$\mathcal{A} u(x_j, t) = \mathcal{B} g(x_j, t) + O(h^4). \tag{36}$$

Combing (12), (35) and (36), one gets

$$\mathcal{B} \cdot \frac{\tau^{-\alpha}}{\Gamma(3-\alpha)} \sum_{i=0}^{k-1} \left[w_{1,k-i}\left(u_j^{i+1} - u_j^{i-1}\right) + w_{2,k-i}\left(u_j^{i+1} - 2u_j^i + u_j^{i-1}\right)\right]$$
$$= \mathcal{A} u_j^k + \mathcal{B} f_j^k + O(\tau^{3-\alpha} + h^4).$$

DOI: 10.1685/journal.caim.536

Using the same assumption and omitting the high-order term, we can obtain a new difference scheme for equation (1) in the following form

(37)
$$\begin{cases} \mathbf{B}\mathbf{U}^1 = \nu(w_{1,k}+w_{2,k})\mathbf{C}\mathbf{U}^0+\mathbf{C}\mathbf{F}^0+\mathbf{G}_1,\ k=1, \\ \mathbf{B}\mathbf{U}^k = \nu(-w_{1,2}+2w_{2,1}-w_{2,2})\mathbf{C}\mathbf{U}^{k-1}-\nu\sum_{i=1}^{k-2}(w_{1,k-i+1}-w_{1,k-i-1} \\ \qquad +w_{2,k-i+1}-2w_{2,k-i}+w_{2,k-i-1})\mathbf{C}\mathbf{U}^i+\nu(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})\mathbf{C}\mathbf{U}^0 \\ \qquad +\mathbf{C}\mathbf{F}^k+\mathbf{G}_k,\ 2\le k\le N, \end{cases}$$

where $\nu=\frac{\tau^{-\alpha}}{\Gamma(3-\alpha)}$, the matrices and vectors in (37) are defined below,

$$\begin{aligned} &\mathbf{B}=\mathrm{tri}\left[s_3,s_2,s_1\right],\ 1\le k\le N,\\ &s_1=\nu(w_{1,1}+w_{2,1})\left(\frac{1}{12}-\frac{V_\alpha h}{24K_\alpha}\right)-\left(\frac{K_\alpha}{h^2}+\frac{V_\alpha^2}{12K_\alpha}-\frac{V_\alpha}{2h}\right),\\ &s_2=\frac{5}{6}\nu(w_{1,1}+w_{2,1})+2\left(\frac{K_\alpha}{h^2}+\frac{V_\alpha^2}{12K_\alpha}\right),\\ &s_3=\nu(w_{1,1}+w_{2,1})\left(\frac{1}{12}+\frac{V_\alpha h}{24K_\alpha}\right)-\left(\frac{K_\alpha}{h^2}+\frac{V_\alpha^2}{12K_\alpha}+\frac{V_\alpha}{2h}\right),\\ &\mathbf{C}=\mathrm{tri}\left[q_3,q_2,q_1\right], \end{aligned}$$

$$\begin{aligned} &q_1=\frac{1}{12}-\frac{V_\alpha h}{24K_\alpha},\\ &q_2=\frac{5}{6},\\ &q_3=\frac{1}{12}+\frac{V_\alpha h}{24K_\alpha},\\ &\mathbf{G}_k=(g_1,\dots,g_{M-1})^T,\\ &g_1=-s_3\varphi(t_k)+q_3\nu(-w_{1,2}+2w_{2,1}-w_{2,2})\varphi(t_{k-1})+q_3\nu(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})\varphi(t_0)\\ &\qquad -q_3\nu\sum_{i=1}^{k-2}(w_{1,k-i+1}-w_{1,k-i-1}+w_{2,k-i+1}-2w_{2,k-i}+w_{2,k-i-1})\varphi(t_i)+q_3f(x_0,t_k),\\ &g_{M-1}=-s_1\psi(t_k)+q_1\nu(-w_{1,2}+2w_{2,1}-w_{2,2})\psi(t_{k-1})+q_1\nu(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})\psi(t_0)\\ &\qquad -q_1\nu\sum_{i=1}^{k-2}(w_{1,k-i+1}-w_{1,k-i-1}+w_{2,k-i+1}-2w_{2,k-i}+w_{2,k-i-1})\psi(t_i)+q_1f(x_M,t_k). \end{aligned}$$

Theorem 4.1. *The difference system (37) has a unique solution.*

Proof. The eigenvalues of the matrix $\mathbf{B}$ are given by

$$\widetilde{\lambda}_i = s_2 + 2\sqrt{s_1 s_3}\ \cos\left(\frac{i}{M}\pi\right),\ i = 1, 2, \ldots, M-1.$$

(i) When $s_1 s_3 = \left[\frac{\nu(4-\alpha)}{24} - \frac{K_\alpha}{h^2} - \frac{V_\alpha^2}{12K_\alpha}\right]^2 - \left[\frac{\nu V_\alpha h(4-\alpha)}{48K_\alpha} - \frac{V-\alpha}{2h}\right]^2 \geq 0$, we have

$$\widetilde{\lambda}_i \geq \frac{5\nu(4-\alpha)}{12} + 2\left(\frac{K_\alpha}{h^2} + \frac{V_\alpha^2}{12K_\alpha}\right) - 2\left|\frac{\nu(4-\alpha)}{24} - \frac{K_\alpha}{h^2} - \frac{V_\alpha^2}{12K_\alpha}\right|.$$

If $\frac{\nu(4-\alpha)}{24} - \frac{K_\alpha}{h^2} - \frac{V_\alpha^2}{12K_\alpha} \geq 0$, then

$$\widetilde{\lambda}_i \geq \frac{\nu(4-\alpha)}{3} + 4\left(\frac{K_\alpha}{h^2} + \frac{V_\alpha^2}{12K_\alpha}\right) > 0,$$

otherwise,

$$\widetilde{\lambda}_i \geq \frac{\nu(4-\alpha)}{2} > 0.$$

(ii) When $s_1 s_3 = \left[\frac{\nu(4-\alpha)}{24} - \frac{K_\alpha}{h^2} - \frac{V_\alpha^2}{12K_\alpha}\right]^2 - \left[\frac{\nu V_\alpha h(4-\alpha)}{48K_\alpha} - \frac{V-\alpha}{2h}\right]^2 < 0$, one has

$$\widetilde{\lambda}_i = \frac{5\nu(4-\alpha)}{12} + 2\left(\frac{K_\alpha}{h^2} + \frac{V_\alpha^2}{12K_\alpha}\right) + 2\widetilde{b}\cos\left(\frac{i}{M}\pi\right)\imath \neq 0,$$

where $\widetilde{b}^2 = \left[\frac{\nu V_\alpha h(4-\alpha)}{48K_\alpha} - \frac{V-\alpha}{2h}\right]^2 - \left[\frac{\nu(4-\alpha)}{24} - \frac{K_\alpha}{h^2} - \frac{V_\alpha^2}{12K_\alpha}\right]^2$.

Therefore, $\mathbf{B}$ is invertible, so the solution exists and is unique. □

Through the above analysis, we easily know that the local truncation error of difference scheme (37) is $\widetilde{R}_j^k = O(\tau^{3-\alpha} + h^4)$.

Next, we give the stability analysis for difference scheme (37).

When $k = 1$

$$s_3\widetilde{\rho}_{j-1}^1 + s_2\widetilde{\rho}_j^1 + s_1\widetilde{\rho}_{j+1}^1 = \frac{\nu(4-\alpha)}{2}\left(q_3\widetilde{\rho}_{j-1}^0 + q_2\widetilde{\rho}_j^0 + q_1\widetilde{\rho}_{j+1}^0\right). \tag{38}$$

When $k > 1$

(39)

$$\begin{aligned} s_3\widetilde{\rho}_{j-1}^k + s_2\widetilde{\rho}_j^k + s_1\widetilde{\rho}_{j+1}^k &= \nu(-w_{1,2} + 2w_{2,1} - w_{2,2})\left(q_3\widetilde{\rho}_{j-1}^{k-1} + q_2\widetilde{\rho}_j^{k-1} + q_1\widetilde{\rho}_{j+1}^{k-1}\right) \\ &- \nu\sum_{i=1}^{k-2}(w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})\left(q_3\widetilde{\rho}_{j-1}^i + q_2\widetilde{\rho}_j^i + q_1\widetilde{\rho}_{j+1}^i\right) \\ &+ \nu(w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})\left(q_3\widetilde{\rho}_{j-1}^0 + q_2\widetilde{\rho}_j^0 + q_1\widetilde{\rho}_{j+1}^0\right). \end{aligned}$$

Let

$$\widetilde{\rho}_j^k = \widetilde{d}_k e^{\imath\sigma jh},$$

and substituting it into (38) and (39) yields

$$\widetilde{d}_1 = \frac{\frac{\nu(4-\alpha)}{2}\left[(q_1+q_3)\cos(\sigma h)+q_2+\imath(q_1-q_3)\sin(\sigma h)\right]}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\,\widetilde{d}_0, \tag{40}$$

and

(41)

$$\begin{aligned}\widetilde{d}_k =& Q\Big\{(-w_{1,2}+2w_{2,1}-w_{2,2})\widetilde{d}_{k-1}+(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})\widetilde{d}_0\\ &-\sum_{i=1}^{k-2}(w_{1,k-i+1}-w_{1,k-i-1}+w_{2,k-i+1}-2w_{2,k-i}+w_{2,k-i-1})\widetilde{d}_i\Big\},\end{aligned}$$

where

$$Q=\frac{\nu[(q_1+q_3)\cos(\sigma h)+q_2+\imath(q_1-q_3)\sin(\sigma h)]}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}.$$

Lemma 4.1. *The following inequality holds*

$$\frac{\nu(4-\alpha)}{2}\left|\frac{[(q_1+q_3)\cos(\sigma h)+q_2+\imath(q_1-q_3)\sin(\sigma h)]}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\right|\leq 1.$$

Proof.

$$\begin{aligned}
&\frac{\nu(4-\alpha)}{2}\left|\frac{[(q_1+q_3)\cos(\sigma h)+q_2+\imath(q_1-q_3)\sin(\sigma h)]}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\right|\leq 1\\
\Leftrightarrow\quad &\frac{\nu(4-\alpha)}{2}\sqrt{[(q_1+q_3)\cos(\sigma h)+q_2]^2+[(q_1-q_3)\sin(\sigma h)]^2}\\
&\leq\sqrt{[(s_1+s_3)\cos(\sigma h)+s_2]^2+[(s_1-s_3)\sin(\sigma h)]^2}\\
\Leftrightarrow\quad &\left[\frac{\nu(4-\alpha)}{2}\right]^2\left\{\left[1-\frac{1}{3}\sin^2\left(\frac{1}{2}\sigma h\right)\right]^2+\left[-\frac{V_\alpha h}{12K_\alpha}\sin(\sigma h)\right]^2\right\}\\
&\leq\left\{\frac{\nu(4-\alpha)}{2}-2\sin^2\left(\frac{1}{2}\sigma h\right)\left[\frac{\nu(4-\alpha)}{12}-2\left(\frac{K_\alpha}{h^2}+\frac{V_\alpha^2}{12K_\alpha}\right)\right]\right\}^2\\
&+\left\{\left[-\frac{V_\alpha h}{12K_\alpha}\cdot\frac{\nu(4-\alpha)}{2}+\frac{V_\alpha}{h}\right]\sin(\sigma h)\right\}^2\\
\Leftrightarrow\quad &\sin^2\left(\frac{\sigma h}{2}\right)\left\{\frac{V_\alpha^2}{h^2}\cos^2\left(\frac{\sigma h}{2}\right)+\frac{4\nu(4-\alpha)K_\alpha}{h^2}\left[1-\frac{1}{3}\sin^2\left(\frac{\sigma h}{2}\right)\right]\right.\\
&\left.+16\sin^2\left(\frac{\sigma h}{2}\right)\left(\frac{K_\alpha}{h^2}+\frac{V_\alpha^2}{12K_\alpha}\right)^2+\frac{\nu(4-\alpha)V_\alpha^2}{6K_\alpha}\left[1+\frac{1}{3}\sin^2\left(\frac{\sigma h}{2}\right)\right]\right\}\geq 0.
\end{aligned}$$

The proof is thus completed. □

Lemma 4.2. *For $\widetilde{d}_k$ $(1 \le k \le N)$ defined by (40) and (41), if $\alpha \in (0, \alpha_1)$, the following inequality*

$$|\widetilde{d}_k| \le |\widetilde{d}_0|$$

holds for $k = 1, 2, ..., N$.

Proof. When $k = 1$, we easily get

$$|\widetilde{d}_1| \le |\widetilde{d}_0|$$

by Lemma 4.1.
When $k = 2$, from Lemma 2.1, if $\alpha \in (0, \alpha_0)$, one can get,

$$|\widetilde{d}_2| \le |\widetilde{d}_0|.$$

Suppose that $|\widetilde{d}_n| \le |\widetilde{d}_0|$ is true for $1 \le n \le k-1$. In view of (41) and Lemma 2.1, if $\alpha \in (0, \alpha_1)$ one has

$$\begin{aligned}
\left|\widetilde{d}_k\right| =& |Q| \left| \Big\{ (-w_{1,2} + 2w_{2,1} - w_{2,2})\widetilde{d}_{k-1} + (w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1})\widetilde{d}_0 \right. \\
& \left. - \sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})\widetilde{d}_i \Big\} \right| \\
\le& |Q| \Big\{ (-w_{1,2} + 2w_{2,1} - w_{2,2}) \left|\widetilde{d}_{k-1}\right| + (w_{1,k} + w_{1,k-1} + w_{2,k} - w_{2,k-1}) \left|\widetilde{d}_0\right| \\
& - \sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1}) \left|\widetilde{d}_i\right| \Big\} \\
\le& |Q| \left(w_{1,1} + w_{2,1}\right) \left|\widetilde{d}_0\right| \\
=& \frac{\nu(4-\alpha)}{2} \left| \frac{[(q_1 + q_3)\cos(\sigma h) + q_2 + \imath(q_1 - q_3)\sin(\sigma h)]}{(s_1 + s_3)\cos(\sigma h) + s_2 + \imath(s_1 - s_3)\sin(\sigma h)} \right| \left|\widetilde{d}_0\right| \\
\le& \left|\widetilde{d}_0\right|.
\end{aligned}$$

The proof is finished. □

Theorem 4.2. *If $\alpha \in (0, \alpha_1)$, the difference scheme (37) is unconditionally stable.*

Proof. In view of Lemma 4.2, one gets

$$\|\widetilde{\rho}^k\|_2^2 = \sum_{m=-\infty}^{\infty} |\widetilde{d}_k(m)|^2 \le \sum_{m=-\infty}^{\infty} |\widetilde{d}_0(m)|^2 = \|\widetilde{\rho}^0\|_2^2,$$

which means that difference scheme (37) is unconditionally stable. □

Finally, we show the convergence analysis.
When $k=1$,
(42)
$$s_3\widetilde{e}_{j-1}^1+s_2\widetilde{e}_j^1+s_1\widetilde{e}_{j+1}^1=\frac{\nu(4-\alpha)}{2}\left(q_3\widetilde{e}_{j-1}^0+q_2\widetilde{e}_j^0+q_1\widetilde{e}_{j+1}^0\right)+\widetilde{R}_j^0,\ j=1,2,...,M-1.$$

When $k>1$,
(43)
$$\begin{aligned}&s_3\widetilde{e}_{j-1}^k+s_2\widetilde{e}_j^k+s_1\widetilde{e}_{j+1}^k=\nu(-w_{1,2}+2w_{2,1}-w_{2,2})\left(q_3\widetilde{e}_{j-1}^{k-1}+q_2\widetilde{e}_j^{k-1}+q_1\widetilde{e}_{j+1}^{k-1}\right)\\&-\nu\sum_{i=1}^{k-2}(w_{1,k-i+1}-w_{1,k-i-1}+w_{2,k-i+1}-2w_{2,k-i}+w_{2,k-i-1})\left(q_3\widetilde{e}_{j-1}^i+q_2\widetilde{e}_j^i+q_1\widetilde{e}_{j+1}^i\right)\\&+\nu(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})\left(q_3\widetilde{e}_{j-1}^0+q_2\widetilde{e}_j^0+q_1\widetilde{e}_{j+1}^0\right)+\widetilde{R}_j^k,\\&j=1,2,...,M-1,\ k=2,3,...,N.\end{aligned}$$

Now, Let
$$\widetilde{e}_j^k=\widetilde{\xi}_k e^{\imath\sigma jh},\ \widetilde{R}_j^k=\widetilde{\eta}_k e^{\imath\sigma jh}.$$
Substituting them into (42) and (43) yields

(44)
$$\begin{aligned}\widetilde{\xi}_1=&\frac{\frac{\nu(4-\alpha)}{2}\left[(q_1+q_3)\cos(\sigma h)+q_2+\imath(q_1-q_3)\sin(\sigma h)\right]}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\widetilde{\xi}_0\\&+\frac{1}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\widetilde{\eta}_1,\end{aligned}$$

and
(45)
$$\begin{aligned}\widetilde{\xi}_k=&Q\Big\{(-w_{1,2}+2w_{2,1}-w_{2,2})\widetilde{\xi}_{k-1}+(w_{1,k}+w_{1,k-1}+w_{2,k}-w_{2,k-1})\widetilde{\xi}_0\\&-\sum_{i=1}^{k-2}(w_{1,k-i+1}-w_{1,k-i-1}+w_{2,k-i+1}-2w_{2,k-i}+w_{2,k-i-1})\widetilde{\xi}_i\Big\}\\&+\frac{1}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\widetilde{\eta}_k.\end{aligned}$$

Lemma 4.3. *The following inequality holds*
$$\left|\frac{1}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\right|\le 2.$$

Proof. Note that $0<\tau<1$ and $0<\alpha<1$, then $1<\Gamma(3-\alpha)<2$ and $\nu=\frac{1}{\tau^{\alpha}\Gamma(3-\alpha)}>\frac{1}{2}$. So,

$$\begin{aligned}
1 &\leq \frac{4}{9}\nu^2(4-\alpha)^2 \leq \nu^2(4-\alpha)^2\left[1-\frac{1}{3}\sin^2\left(\frac{1}{2}\sigma h\right)\right]^2\\
&= 4\left\{\left[\frac{\nu(4-\alpha)}{2}\right]\left[1-\frac{1}{3}\sin^2\left(\frac{1}{2}\sigma h\right)\right]\right\}^2\\
&\leq 4\left\{\frac{\nu(4-\alpha)}{2}-2\sin^2\left(\frac{1}{2}\sigma h\right)\left[\frac{\nu(4-\alpha)}{12}-2\left(\frac{K_\alpha}{h^2}+\frac{V_\alpha^2}{12K_\alpha}\right)\right]\right\}^2\\
&\quad+4\left\{\left[-\frac{V_\alpha h}{12K_\alpha}\cdot\frac{\nu(4-\alpha)}{2}+\frac{V_\alpha}{h}\right]\sin(\sigma h)\right\}^2\\
&= 4\left|(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)\right|^2,
\end{aligned}$$

i.e.,

$$\left|\frac{1}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\right|\leq 2.$$

The proof is finished. □

Lemma 4.4. *For $\widetilde{\xi}_k$ $(k=1,2,...,N)$ given by (44) and (45), if $\alpha\in(0,\alpha_1)$, then there exists a positive constant $\widetilde{C}_2$ such that*

$$|\widetilde{\xi}_k|\leq \widetilde{C}_2(1+\tau)^k|\widetilde{\eta}_1|, k=1,2,...,N.$$

Proof. Similar to the preceding proof, one has

$$|\widetilde{\eta}_k|\equiv|\widetilde{\eta}_k(m)|\leq\frac{1}{2}\widetilde{C}_2\tau|\widetilde{\eta}_1|\equiv\frac{1}{2}\widetilde{C}_2\tau|\widetilde{\eta}_1(m)|, k=1,2,...,N. \tag{46}$$

Using $\widetilde{\xi}_0=0$, (44) and Lemma 4.3, gives

$$\begin{aligned}
\left|\widetilde{\xi}_1\right| &= \left|\frac{1}{(s_1+s_3)\cos(\sigma h)+s_2+\imath(s_1-s_3)\sin(\sigma h)}\right||\widetilde{\eta}_1|\\
&\leq 2\left|\widetilde{\eta}_1\right|\leq\widetilde{C}_2\tau|\widetilde{\eta}_1|\leq(1+\tau)\widetilde{C}_2|\widetilde{\eta}_1|.
\end{aligned}$$

When $k=2$, from Lemma 2.1, if $\alpha\in(0,\alpha_0)$, one get

$$|\widetilde{\xi}_2|\leq(1+\tau)^2\widetilde{C}_2|\widetilde{\eta}_1.$$

Now, we suppose that

$$\left|\widetilde{\xi}_n\right|\leq(1+\tau)^n\widetilde{C}_2\left|\widetilde{\eta}_1\right|,\ n=1,2,\ldots,k-1.$$

Using (45), Lemmas 4.1, 4.3 and 2.1 again, if $\alpha \in (0, \alpha_1)$, it is easy to get

$$\begin{aligned}
\left|\widetilde{\xi}_k\right| \le& |Q| \Big\{ (-w_{1,2} + 2w_{2,1} - w_{2,2}) \left|\widetilde{\xi}_{k-1}\right| \\
&- \sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1}) \left|\widetilde{\xi}_i\right| \Big\} \\
&+ \left| \frac{1}{(s_1 + s_3)\cos(\sigma h) + s_2 + \imath(s_1 - s_3)\sin(\sigma h)} \right| |\widetilde{\eta}_k| \\
\le& |Q| \Big\{ (-w_{1,2} + 2w_{2,1} - w_{2,2})(1+\tau)^{k-1} \widetilde{C}_2 |\widetilde{\eta}_1| \\
&- \sum_{i=1}^{k-2} (w_{1,k-i+1} - w_{1,k-i-1} + w_{2,k-i+1} - 2w_{2,k-i} + w_{2,k-i-1})(1+\tau)^i \widetilde{C}_2 |\widetilde{\eta}_1| \Big\} + 2 |\widetilde{\eta}_k| \\
\le& |Q| (w_{1,1} + w_{2,1}) (1+\tau)^{k-1} \widetilde{C}_2 |\widetilde{\eta}_1| + \tau \widetilde{C}_2 |\widetilde{\eta}_1| \\
\le& (1+\tau)^{k-1} \widetilde{C}_2 |\widetilde{\eta}_1| + \tau \widetilde{C}_2 |\widetilde{\eta}_1| \\
\le& (1+\tau)^k \widetilde{C}_2 |\widetilde{\eta}_1| .
\end{aligned}$$

This ends the proof. □

Theorem 4.3. *If $\alpha \in (0, \alpha_1)$, the finite difference scheme (37) is L2-convergent with order $O(\tau^{3-\alpha} + h^4)$.*

Proof. Similar to the proof of Theorem 3.4, it follows that

$$\|\widetilde{e}^k\|_2 \le (1+\tau)^k \widetilde{C}_2 \|\widetilde{R}^1\|_2 \le e^{k\tau} \widetilde{C}_1 \widetilde{C}_2 \sqrt{L} (\tau^{3-\alpha} + h^4) \le \widetilde{C} (\tau^{3-\alpha} + h^4). \quad \square$$

5. Numerical examples

In this section, the numerical examples are presented to illustrate our theoretical analysis. Example 5.1 is used to verify the numerical scheme for Caputo derivative. Example 5.2 is displayed to test numerical schemes I and II.

Example 5.1. Consider the function $f(t) = t^4, t \in [0, 1]$.

The numerical results are shown in Table 1. From this table, the experiment convergence order is in line with the theoretical order $(3 - \alpha)$.

In the following, we apply numerical schemes I and II to compute the following fractional partial differential equation.

Table 1. The absolute error, convergence order of Example 5.1 by numerical scheme (9).

α	τ	the absolute error	the convergence order
0.2	$\frac{1}{10}$	0.0015	—
	$\frac{1}{20}$	2.4095e-04	2.6382
	$\frac{1}{40}$	3.7575e-05	2.6809
	$\frac{1}{80}$	5.7436e-06	2.7097
	$\frac{1}{160}$	8.6640e-07	2.7289
0.4	$\frac{1}{10}$	0.0052	—
	$\frac{1}{20}$	9.3209e-04	2.4800
	$\frac{1}{40}$	1.6158e-04	2.5282
	$\frac{1}{80}$	2,7540e-05	2.5526
	$\frac{1}{160}$	4.6455e-06	2.5676
0.6	$\frac{1}{10}$	0.0139	—
	$\frac{1}{20}$	0.0028	2.3116
	$\frac{1}{40}$	5.4517e-04	2.3606
	$\frac{1}{80}$	1.0520e-04	2.3736
	$\frac{1}{160}$	2.0146e-05	2.3846
0.8	$\frac{1}{10}$	0.0331	—
	$\frac{1}{20}$	0.0075	2.1419
	$\frac{1}{40}$	0.0017	2.1414
	$\frac{1}{80}$	3.6991e-04	2.2003
	$\frac{1}{160}$	8.1011e-05	2.1910

Example 5.2. Consider the time fractional advection-diffusion equation in the following form

$$\begin{cases} {}_C D_{0,t}^{\alpha} u(x,t) = \dfrac{\partial^2 u(x,t)}{\partial x^2} - \dfrac{\partial u(x,t)}{\partial x} + f(x,t), \ x \in (0,1), \ t > 0, \\ u(x,0) = 0, \ 0 \leq x \leq 1, \\ u(0,t) = 0, \ u(1,t) = 0, \ t > 0, \end{cases} \tag{47}$$

in which $f(x,t) = \frac{\Gamma(6) t^{5-\alpha}}{\Gamma(6-\alpha)} \sin(\pi x) + \pi t^5 (\pi \sin(\pi x) + \cos(\pi x))$. Its analytical solution is $u(x,t) = t^5 \sin(\pi x)$.

Here let $T = 1$. We find its numerical solution in $(x,t) \in [0,1] \times [0,1]$. The absolute error, time and space convergence orders are listed in Tables 2, 3 and 4 by difference schemes (15) and (37). From these tables, we can see that the numerical results coincide with the theoretical convergence orders.

DOI: 10.1685/journal.caim.536

Table 2. The absolute error, time convergence order of Example 5.2 by difference scheme (15) with $h = \frac{1}{1000}$.

α	τ	the absolute error	the time convergence order
0.1	$\frac{1}{10}$	1.1114e-04	—
	$\frac{1}{12}$	6.9539e-05	2.5721
	$\frac{1}{14}$	4.6663e-05	2.5869
	$\frac{1}{16}$	3.3006e-05	2.5940
	$\frac{1}{18}$	2.4329e-05	2.5891
0.2	$\frac{1}{10}$	2.9151e-04	—
	$\frac{1}{12}$	1.8413e-04	2.5200
	$\frac{1}{14}$	1.2440e-04	2.5428
	$\frac{1}{16}$	8.8389e-05	2.5603
	$\frac{1}{18}$	6.5313e-05	2.5688
0.37	$\frac{1}{10}$	8.6553e-04	—
	$\frac{1}{12}$	5.5877e-04	2.4004
	$\frac{1}{14}$	3.8437e-04	2.4261
	$\frac{1}{16}$	2.7726e-04	2.4464
	$\frac{1}{18}$	2.0751e-04	2.4601

Table 3. The absolute error, space convergence order of Example 5.2 by difference scheme (15) with $\tau = \frac{1}{200}$.

α	h	the absolute error	the space convergence order
0.1	$\frac{1}{2}$	0.2035	—
	$\frac{1}{4}$	0.0479	2.0869
	$\frac{1}{8}$	0.0118	2.0212
	$\frac{1}{16}$	0.0030	1.9758
0.2	$\frac{1}{2}$	0.1988	—
	$\frac{1}{4}$	0.0470	2.0806
	$\frac{1}{8}$	0.0116	2.0185
	$\frac{1}{16}$	0.0029	2.0000
0.37	$\frac{1}{2}$	0.1895	—
	$\frac{1}{4}$	0.0451	2.0710
	$\frac{1}{8}$	0.0111	2.0226
	$\frac{1}{16}$	0.0028	1.9871

6. Conclusions

In this paper, we give a $(3-\alpha)$th-order numerical method to approximate the Caputo derivative, where $\alpha \in (0,1)$. Using this scheme, propose two numerical schemes with convergence order $O(\tau^{3-\alpha} + h^2)$ and $O(\tau^{3-\alpha}+h^4)$ for time fractional advection-diffusion equation, where τ, h are time steplength and space steplength, respectively. The stability of the derived numerical algorithms are proved by the Fourier method. Here we must pay attention that the unconditional stability depend upon the derivative order α. The numerical results support the theoretical analysis.

Table 4. The absolute error, space convergence order of Example 5.2 by difference scheme (37) with $\tau = \frac{1}{1000}$.

α	h	the absolute error	the space convergence order
0.1	$\frac{1}{10}$	3.3278e-05	—
	$\frac{1}{12}$	1.61051e-05	3.9995
	$\frac{1}{14}$	8.6486e-06	4.0104
	$\frac{1}{16}$	5.0579e-06	4.0180
	$\frac{1}{18}$	3.1587e-06	3.9966
0.2	$\frac{1}{10}$	3.2703e-05	—
	$\frac{1}{12}$	1.5769e-05	4.0011
	$\frac{1}{14}$	8.4954e-06	4.0110
	$\frac{1}{16}$	4.9679e-06	4.0187
	$\frac{1}{18}$	3.1053e-06	3.9890
0.37	$\frac{1}{10}$	3.1553e-05	—
	$\frac{1}{12}$	1.5209e-05	4.0033
	$\frac{1}{14}$	8.1925e-06	4.0123
	$\frac{1}{16}$	4.7914e-06	4.0180
	$\frac{1}{18}$	3.0018e-06	3.9694

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