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Research Article

Efficient Evaluation of the Liouville-Caputo Fractional Derivative for TFCRD Equations

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Abstract: For the variable coefficient Time-Fractional Convection-Reaction-Diffusion (TFCRD) equation, a fast compact finite difference scheme based on an efficient and high-order accurate numerical formulation to accelerate the computation of Liouville-Caputo derivatives is presented. The proposed method led to speed up the evaluation of the Liouville-Caputo fractional derivative based on the $L2-1_\delta$ when compared to the numerical solution of the variable coefficient TFCRD equation given by directly evaluating $L2-1_\delta$ formula. The proposed difference scheme not only maintains unconditional stability and high accuracy, but also significantly reduces storage requirements and computational costs. Numerical experiments confirm the theoretical analysis.

***Keywords*:** Time-Fractional Convection-Reaction-Diffusion (TFCRD) equation, sum of exponentials, stability and convergence, fast algorithm

MSC: 65M06, 65M12, 65M15, 35R11

1. Introduction

Fractional calculus has emerged as a powerful mathematical tool for modeling anomalous diffusion phenomena [1–13]. Among various fractional operators, the Liouville-Caputo fractional derivative has gained particular prominence due to its compatibility with standard initial conditions in differential equations. Recent advances in computational fractional calculus have enabled the numerical treatment of time-fractional convection-reaction-diffusion equations, which constitute a class of equations that effectively capture memory-dependent transport processes in heterogeneous media [14–27]. In the above literatures, Bueno-Orovio et al. proposed fractional diffusion models as a novel mathematical description of structurally heterogeneous excitable media [14], Cui gave a compact exponential scheme for the variable coefficient Time-Fractional Convection-Reaction-Diffusion (TFCRD) equation [16], Gao et al. proposed a high-order accurate three-point combined compact difference scheme with the $L1$ formula to solve a class of time-fractional advection-diffusion equations [17], Li et al. studied the time-space fractional order nonlinear subdiffusion and superdiffusion equations, which can relate the matter flux vector to concentration gradient in the general sense [18]. Liu et al. proposed computationally effective implicit numerical methods for these fractional advection-dispersion models [19]. In [21], Lv and Xu proposed and analyzed a fractional spectral method for the time-fractional diusion equation. Vong et al. proposed a scheme and

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showed that it converges with second order in time and fourth order in space, the accuracy of proposed method can be improved by Richardson extrapolation [24]. In [26], a novel implicit numerical method for the time variable fractional order mobile-immobile advection-dispersion is proposed and the stability of the approximation is investigated. Zhao and Deng developed a series of high-order quasi-compact schemes for space fractional diffusion equations [27].

Despite theoretical advances, significant computational challenges remain in implementing Liouville-Caputo derivative-based models. The historical dependence of fractional operators induces prohibitive $O(N^2)$ computational complexity and $O(N)$ storage requirements for N temporal steps, particularly detrimental for long-time simulations of variable coefficient systems. While existing approximation methods (e.g., $L2-1_\delta$ formula [15]) provide certain accuracy improvements, they generally suffer from either limited convergence rates or insufficient stability guarantees when coupled with spatial discretization schemes. This motivates the development of novel computational frameworks that simultaneously address accuracy, efficiency, and implementation practicality.

Substantial research efforts in the literature have been devoted to accelerating the computation of weakly singular integral kernels. Lubich and Schadle proposed a fast convolution for non-reflecting boundary conditions [28]. The Sum-of-Exponentials (SOE) [29] approximation for $t^{-\beta}$ on $[\delta, T]$ for $\beta \in (0, 2)$ as follows

$$\left| t^{-\beta} - \left(\sum_{k=1}^{m_0} e^{-t_{0,k}p} w_{0,k} + \sum_{j=-N}^{-1} \sum_{k=1}^{m_s} e^{-t_{j,k}p} s_{j,k}^{\beta-1} w_{j,k} + \sum_{j=0}^{M} \sum_{k=1}^{m_l} e^{-t_{j,k}p} s_{j,k}^{\beta-1} w_{j,k} \right) \right| \le \varepsilon,$$

where $m_0 = O\left(\log \frac{1}{\varepsilon}\right)$, $N = O(\log T)$, $M = O\left(\log\log \frac{1}{\varepsilon} + \log \frac{1}{\delta}\right)$, and $t_{0,1}, \cdots, t_{0,m_0}$, $w_{0,1}, \cdots, w_{0,m_0}$ be the nodes and weights for the m_0-point Gauss-Jacobi quadrature on the interval $[0, 2^{-N}]$, $s_{j,1}, \cdots, s_{j,m_s}$ and $w_{j,1}, \cdots, w_{j,m_s}$ be the nodes and weights. The fast algorithm keeps the accuracy of $O(\tau^{2-\alpha})$ with the $L1$ formula, meanwhile, reduces the computational complexity. More discussion on approximations the kernel functions of Sum-of-Exponentials can be referenced [30–33].

This study focuses on the variable-coefficient TFCRD equations. The complete mathematical framework, including the governing equations, boundary conditions, and initial conditions, is formally defined in system

$$\begin{cases} {}_0^C\mathscr{D}_t^\alpha u(x, t) = \dfrac{\partial^2 u}{\partial x^2}(x, t) - \beta_1(x)\dfrac{\partial u}{\partial x}(x, t) + \beta_2(x)u(x, t) + f(x, t), \qquad (x, t) \in (0, L) \times (0, T), \\ u(0, t) = \psi_0(t), \quad u(L, t) = \psi_L(t), \qquad t \in (0, T], \\ u(x, 0) = \phi(x), \qquad x \in [0, L], \end{cases} \tag{1}$$

where the term ${}_0^C\mathscr{D}_t^\alpha u(x, t)$ represents the Liouville-Caputo time-fractional derivative of order α $(0 < \alpha < 1)$, which is defined by

$${}_0^C\mathscr{D}_t^\alpha u(x, t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{u'(x, s)}{(t-s)^\alpha} \mathrm{d}s, \qquad 0 < \alpha < 1. \tag{2}$$

In this paper, we suppose $\beta_1(x)$, $\beta_2(x)$, f, $\psi_0(t)$, $\psi_L(t)$ and $\phi(x)$ in (1) are smooth enough. Combining the $L2-1_\delta$ formula with the SOE approximation to produce a fast evaluation formula for the time fractional derivative (called $FL2-1_\delta$), which defined by ${}^{FH}D_t^\alpha$ given as

$$ {}^{FH}D_t^{\alpha} v^{n+\delta} = \sum_{i=1}^{N_{exp}} \hat{w}_i \hat{V}_i^n + \frac{1}{\Gamma(1-\alpha)} \frac{v^{n+1}-v^n}{\tau} \int_{t_n}^{t_{n+\delta}} \frac{1}{(t_{n+\delta}-s)^{\alpha}} ds, $$

which $\hat{V}_i^n$ is evaluated by the recurrence relation $\hat{V}_i^n = e^{-s_i \tau} \hat{V}_i^{n-1} + A_i(v^n - v^{n-1}) + B_i(v^{n+1} - v^n)$ [34]. In this paper, the proposed method reduces significantly the computational complexity comparing with directly evaluating $L2-1_{\delta}$ formula in the paper [35–37] mentioned previously for different TFCRD equations.

Now, we briefly explain the methods $L1/L2/L2-1_{\delta}$ as follows.

$$ L1\text{:}\ \ {}_0^C D_t^{\alpha} u(t_n) = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} [u(t_{k+1}) - u(t_k)] \left[(n-k)^{1-\alpha} - (n-k-1)^{1-\alpha}\right] + O(\tau^2), $$

$$ L2\text{:}\ \ {}_0^C D_t^{\alpha} u(t_n) = \frac{\tau^{-\alpha}}{\Gamma(2-\alpha)} \sum_{k=0}^{n-1} [a_{n-k-1} u(t_{k+1}) - (a_{n-k-1} + a_{n-k}) u(t_k) + a_{n-k} u(t_{k-1})] + O(\tau^{3-\alpha}), $$

$$ L2-1_{\delta}\text{:}\ \ {}_0^C D_t^{\alpha} u\left(t_{n-\frac{\alpha}{2}}\right) = \frac{1}{\tau^{\alpha} \Gamma 2-\alpha} + \sum_{k=1}^{n} c_{n-k,\,n}^{(\alpha)} (w(t_k) - w(t_{k-1})) + O(\tau^{3-\alpha}). $$

Although there are fast algorithms for fractional derivatives (such as SOE), there is still relatively little work on applying them to high-order compact finite difference schemes for variable coefficient TFCRD equations. The motivation of this paper is to construct a class of efficient, stable, and high-precision numerical methods for the TFCRD equations using the $L2-1_{\delta}$ formula and a fast time fractional order algorithm.

The paper proceeds as follows: Section 2 describes a fast Liouville-Caputo derivative evaluation method. Compact difference schemes for variable-coefficient TFCRD equations are developed in Section 3. Section 4 presents stability and convergence analyses. Numerical validations follow in Section 5. Concluding remarks are given in Section 6.

2. Fast evaluation of the Liouville-Caputo fractional derivative

Let

$$ \gamma(x) = e^{\left(-\frac{1}{2}\int_0^x \beta_1(s)\mathrm{d}s\right)}, \quad w(x,\,t) = \gamma(x) u(x,\,t), \quad g(x,\,t) = \gamma(x) f(x,\,t). $$

where $\beta_1(x)$ is differentiable in $x \in [0,\,L]$. For convenience, we use w, u, g to represent $w(x,\,t)$, $u(x,\,t)$, $g(x,\,t)$ respectively.

Multiplying both sides of equation (1) by $\gamma(x)$, we have

$$ {}_0^C\mathscr{D}_t^{\alpha} w(x,\,t) = \gamma(x) \frac{\partial^2 u}{\partial x^2}(x,\,t) - \beta_1(x)\gamma(x) \frac{\partial u}{\partial x}(x,\,t) + \beta_2(x) w(x,\,t) + g(x,\,t). \tag{3} $$

Since $w(x,\,t) = \gamma(x) u(x,\,t)$ and

$$\gamma'(x) = -\frac{1}{2}\gamma(x)\beta_1(x), \qquad \gamma''(x) = \frac{1}{2}\gamma(x)\left(\frac{\beta_1^2(x)}{2} - \beta_1'(x)\right),$$

Derive $w(x, t) = \gamma(x)u(x, t)$ twice, and substitute the above equations into, we obtain

$$\frac{\partial^2 w}{\partial x^2} = \gamma(x)\frac{\partial^2 u}{\partial x^2} - \beta_1(x)\gamma(x)\frac{\partial u}{\partial x} + \frac{1}{2}\left(\frac{\beta_1^2(x)}{2} - \beta_1'(x)\right)w,$$

By organizing the above equation, we can obtain

$$\gamma(x)\frac{\partial^2 u}{\partial x^2} - \beta_1(x)\gamma(x)\frac{\partial u}{\partial x} = \frac{\partial^2 w}{\partial x^2} + \frac{1}{2}\left(\beta_1'(x) - \frac{\beta_1^2(x)}{2}\right)w.$$

Substituting the above equality into (3) yields

$${}_0^C\mathscr{D}_t^\alpha w = \frac{\partial^2 w}{\partial x^2} + \rho(x)w + g,$$

where

$$\rho(x) = \beta_2(x) + \frac{1}{2}\beta_1'(x) - \frac{\beta_1^2(x)}{4}.$$

Therefore, problem (1) can be transformed into

$$\begin{cases} {}_0^C\mathscr{D}_t^\alpha w(x, t) = \dfrac{\partial^2 w}{\partial x^2}(x, t) + \rho(x)w(x, t) + g(x, t), \quad (x, t) \in (0, L) \times (0, T), \\ w(0, t) = \psi_0^*(t), \;\; w(L, t) = \psi_L^*(t), \quad t \in (0, T], \\ w(x, 0) = \phi^*(x). \end{cases} \tag{4}$$

where $\psi_0^*(t) = \psi_0(t)$, $\psi_L^*(t) = \gamma(L)\psi_L(t)$ and $\phi^*(x) = \gamma(x)\phi(x)$.

Let $t_n = n\tau$ and $t_{n-\frac{\alpha}{2}} = \left(n - \dfrac{\alpha}{2}\right)\tau$, which $\tau = T/N$ be the time step, $h = L/M$ be the spatial step, $x_i = ih$ $(0 \le i \le M)$. Define difference operators as follows

$$\zeta_x z_{i-\frac{1}{2}} = (z_i - z_{i-1})/h, \quad \zeta_x^2 z_i = (z_{i+1} - 2z_i + z_{i-1})/h^2, \quad \mathscr{S}_x z_i = z_i + h^2\zeta_x^2 z_i/12,$$

$$\delta_t\zeta^{n-1/2} = \frac{\zeta^n - \zeta^{n-1}}{\tau}, \quad \sigma = 1 - \frac{\alpha}{2}, \quad \vartheta_k = k + \sigma, \quad a_0^{(\alpha)} = \vartheta_0^{1-\alpha}. \tag{5}$$

Lemma 1 Let $\zeta(x) \in \mathscr{C}^6[0, L]$. We have

$$\mathscr{S}_x \left(\frac{\mathrm{d}^2\zeta}{\mathrm{d}x^2} \right)(x_i) = \delta_x^2 \zeta(x_i) + R(x_i), \quad i \in (1, M-1), \tag{6}$$

where

$$R(x_i) = \frac{h^4}{360} \int_0^1 \left(\frac{\partial^6 \zeta}{\partial x^6}(x_i + mh) + \frac{\partial^6 \zeta}{\partial x^6}(x_i - mh) \right) \zeta(m) \mathrm{d}m, \tag{7}$$

with $\zeta(m) = 5(1-m)^3 - 3(1-m)^5$.

Proof. See, e.g., [33]. □

Lemma 2 [34] For $\alpha \in (0, 1)$, there exist positive integer N, s_i and weights w_i $(i = 1, 2, \cdots, \mathbb{N})$ satisfying

$$\left| \frac{1}{t^\alpha} - \sum_{i=1}^{N} w_i e^{-s_i t} \right| \leq \varepsilon, \quad \forall t \in [\tilde{\tau}, T], \tag{8}$$

where ε is tolerance error, $\tilde{\tau}$ is cut-off time step size.

According to approximate $(t_{n+\sigma} - s)^{-\alpha}$ in the Liouville-Caputo fractional derivative by SOE, we now deduce the $FL2-1_\delta$ formula as follows

$$\begin{aligned}
&{}_0^C\mathscr{D}_t^\alpha \zeta(t_{n+\sigma}) \\
&\approx \frac{1}{\Gamma(1-\alpha)} \left(\int_0^{t_n} \zeta'(s) \sum_{i=1}^{\mathbb{N}} w_i e^{-s_i(t_{n+\sigma}-s)} ds + \int_{t_n}^{t_{n+\sigma}} \frac{(\Theta_{1,n}\zeta(s))'}{(t_{n+\sigma}-s)^\alpha} ds \right) \\
&= \sum_{i=1}^{\mathbb{N}} \frac{w_i}{\Gamma(1-\alpha)} \int_0^{t_n} \zeta'(s) e^{-s_i(t_{n+\delta}-s)} ds + \frac{\zeta^{n+1} - \zeta^n}{\tau\Gamma(1-\alpha)} \int_{t_n}^{t_{n+\sigma}} \frac{1}{(t_{n+\sigma}-s)^\alpha} ds \\
&= \sum_{i=1}^{\mathbb{N}} \tilde{w}_i Z_i^n + \frac{a_0^{(\alpha)}}{\mu} (\zeta^{n+1} - \zeta^n),
\end{aligned}$$

where

$$\mu = \tau^\alpha \Gamma(2-\alpha), \quad \tilde{w}_i = w_i / \Gamma(1-\alpha), \quad Z_i = \int_0^{t_n} \frac{\zeta'(s)}{e^{s_i(t_{n+\sigma}-s)}} ds, \quad \Theta_{1,n}\zeta(t) = \zeta^n \frac{t_{n+1}-t}{\tau} + \zeta^{n+1} \frac{t-t_n}{\tau}.$$

The term Z_i^n in this formulation corresponds to the historical integral component, which is computed through a recursive algorithm combined with quadratic interpolation, specifically expressed as

$$Z_i = \int_0^{t_n} \frac{\zeta'(s)}{e^{s_i(t_{n+\sigma}-s)}} ds$$

$$\approx \int_{t_0}^{t_{n-1}} \frac{\zeta'(s)}{e^{s_i(t_{n+\sigma}-s)}} ds + \int_{t_{n-1}}^{t_n} \frac{(\Theta_{2,\,n}\zeta(t))'}{e^{s_i(t_{n+\sigma}-s)}} ds$$

$$= e^{-s_i\tau} Z_i^{n-1} + \kappa_i \tau \delta_t \zeta^{n-1/2} + \xi_i \tau \delta_t \zeta^{n+1/2}$$

with

$$\kappa_i = \int_0^1 \frac{(3/2 - s)}{e^{s_i\tau(\sigma+1-s)}} ds, \quad \xi_i = \int_0^1 \frac{(s-1/2)}{e^{s_i\tau(\sigma+1-s)}} ds,$$

$$\Theta_{2,\,n}\zeta(t) = \zeta^{n-1} \frac{t^2 - (t_n + t_{n+1})t + t_n t_{n+1}}{2\tau^2} - \zeta^n \frac{t^2 - (t_{n-1} + t_{n+1})t + t_{n-1}t_{n+1}}{\tau^2} + \zeta^{n+1} \frac{t^2 - (t_n + t_{n-1})t + t_n t_{n-1}}{2\tau^2}.$$

In composite, the $FL2-1_\delta$ computational operator is architecturally defined by

$${}_0^{FC}\mathscr{D}_t^\alpha \zeta^{n+\sigma} = \sum_{i=1}^{\mathbb{N}} \tilde{w}_i \tilde{Z}_i^n + \frac{\delta_t \zeta^{n+1/2}}{\Gamma(1-\alpha)} \int_{t_n}^{t_{n+\delta}} (t_{n+\delta} - s)^{-\alpha} ds,$$

where

$$\tilde{Z}_i^n = e^{-s_i\tau} \tilde{Z}_i^{n-1} + \kappa_i \tau \delta_t \zeta^{n-1/2} + \xi_i \tau \delta_t \zeta^{n+1/2}, \tag{9}$$

with $\tilde{Z}_i^0 = 0$ $(i = 1, \cdots, \mathbb{N})$.

To facilitate rigorous stability and convergence analysis, the recursive formulation (9) governing $\tilde{Z}_i^n$ admits an equivalent summation representation

$$\tilde{Z}_i^n = e^{-(n-1)s_i\tau} \kappa_i (\zeta^1 - \zeta^0) + \sum_{j=1}^{n-1} \left(\frac{\kappa_i}{e^{(n-j-1)s_i\tau}} + \frac{\xi_i}{e^{(n-j)s_i\tau}} \right) (\zeta^{j+1} - \zeta^j) + \xi_i (\zeta^{n+1} - \zeta^n),$$

which leads to

$${}_0^{FC}\mathscr{D}_t^\alpha \zeta^{n+\sigma} = \sum_{i=1}^{\mathbb{N}} \tilde{w}_i \left[e^{-(n-1)s_i\tau} \kappa_i (\zeta^1 - \zeta^0) + \sum_{k=1}^{n-1} \left(\frac{\kappa_i}{e^{(n-k-1)s_i\tau}} + e^{-(n-k)s_i\xi_i} \right) (\zeta^{k+1} - \zeta^k) + \xi_i (\zeta^{n+1} - \zeta^n) \right]$$

$$+ \frac{a_0^{(\alpha)}}{\mu} (\zeta^{n+1} - \zeta^n) = \sum_{k=0}^{n} (\zeta^{k+1} - \zeta^k) \Upsilon_k^{n+1},$$

where $\Upsilon_0^1 = a_0^{(\alpha)}/\mu$ and

$$\Upsilon_k^{n+1} = \begin{cases} \sum_{i=1}^{\mathbb{N}} \frac{\tilde{w}_i \kappa_i}{e^{(n-1)s_i\tau}}, & k = 0, \\ \sum_{i=1}^{\mathbb{N}} \tilde{w}_i \left(\frac{\kappa_i}{e^{-(n-k-1)s_i\tau}} + \frac{\xi_i}{e^{(n-k)s_i\tau}} \right), & k \in (1, n-1). \\ \sum_{i=1}^{\mathbb{N}} \tilde{w}_i \xi_i + a_0^{(\alpha)}/\mu, & k = n. \end{cases} \tag{10}$$

Lemma 3 [34] For any $\alpha \in (0, 1)$ and $\zeta(t) \in \mathscr{C}^3[0, t_N]$, it holds that

$${}_0^C\mathscr{D}_t^\alpha \zeta(t_{n+\sigma}) = {}_0^{FC}\mathscr{D}_t^\alpha \zeta^{n+\sigma} + \mathscr{O}(\tau^{3-\alpha} + \varepsilon), \quad n = 0, 1, \cdots, N-1.$$

Lemma 4 For any $w(t) \in C^2[0, T]$, then for $n \geq 1$, it holds that

$$w\left(t_{n-\frac{\alpha}{2}}\right) = \frac{\alpha}{2} w(t_{n-1}) + \left(1 - \frac{\alpha}{2}\right) w(t_n) + O(\tau^2).$$

Proof. For function $w(t)$, performing Taylor expansion for $t = t_{n-1}$ and $t = t_n$ at point $t_{n-\frac{\alpha}{2}}$ to obtain the above result. □

3. Compact difference schemes for TFCRD equations

Leveraging the established theoretical foundations in above lemmas, we rigorously formulate a high-order compact discretization of equation (4), yielding a compact difference scheme. We define

$$\delta_t w^{n-\frac{1}{2}} = \frac{1}{\tau}\left(w^n - w^{n-1}\right), \qquad w^{n, \frac{\alpha}{2}} = \frac{\alpha}{2} w^{n-1} + \left(1 - \frac{\alpha}{2}\right) w^n \ \ (n \in (1, N)),$$

$$W_i^n = w(x_i, t_n), \qquad Z_i^n = \frac{\partial^2 w}{\partial x^2}(x_i, t_n), \qquad q_i = q(x_i),$$

$$g_i^{n-\frac{\alpha}{2}} = g\left(x_i, t_{n-\frac{\alpha}{2}}\right), \qquad \phi_0^{*,n} = \phi_0^*(t_n), \qquad \phi_L^{*,n} = \phi_L^*(t_n), \qquad \varphi_i^* = \varphi^*(x_i),$$

$$\delta_x^2 w_i = (w_{i+1} - 2w_i + w_{i-1})/h^2, \qquad S_x = \left(I + \frac{h^2}{12}\delta_x^2\right) w_i.$$

where $w = \{w^n \mid 0 \leq n \leq N\}$ is a given grid function. Applying the governing operator of equation (4) at the point $\left(x_i, t_{n-\frac{\alpha}{2}}\right)$, we obtain

$$
{}_{0}^{FC}\mathscr{D}_t^{\alpha} w\left(x_i, t_{n-\frac{\alpha}{2}}\right) = Z_i^{n-\frac{\alpha}{2}} + q_i W_i^{n-\frac{\alpha}{2}} + g_i^{n-\frac{\alpha}{2}}. \tag{11}
$$

Then we discretize the equation, from the above Lemmas, we obtain

$$
\frac{1}{\mu}\sum_{k=1}^{n} \Upsilon_k^n \mathscr{S}_x\left(W_i^k - W_i^{k-1}\right) = \delta_x^2 W_i^{n,\frac{\alpha}{2}} + \mathscr{S}_x\left(q_i W_i^{n,\frac{\alpha}{2}}\right) + \mathscr{S}_x g_i^{n-\frac{\alpha}{2}} + ({}^F R_{tx}^{\alpha})_i^n, \tag{12}
$$

where

$$
|({}^F R_{tx}^{\alpha})_i^n| \leq C_F(\tau^2 + h^4 + \varepsilon), \quad i \in [1, M-1], \quad n \in [1, N].
$$

with a positive constant C_F. Omitting $({}^F R_{tx}^{\alpha})_i^n$, the compact finite difference scheme as follows

$$
\begin{cases}
\dfrac{1}{\mu}\displaystyle\sum_{k=1}^{n} \Upsilon_k^n \mathscr{S}_x\left(w_i^k - w_i^{k-1}\right) = \delta_x^2 w_i^{n,\frac{\alpha}{2}} + \mathscr{S}_x\left(q_i w_i^{n,\frac{\alpha}{2}}\right) + \mathscr{H}_x g_i^{n-\frac{\alpha}{2}}, \quad i \in [1, M-1], \quad n \in [1, N], \\
w_0^n = \psi_0^{*,n}, \quad w_M^n = \psi_L^{*,n}, \\
w_i^0 = \phi_i^*,
\end{cases} \tag{13}
$$

where w_i^n is the discretized approximation of the solution W_i^n.

4. Stability and convergence of (13)

The stability and convergence properties of the scheme (13) are rigorously analyzed through a novel analytical framework that enables precise error estimation in discrete L^2-norm spaces.

Let grid function $\mathscr{S}_h = \{w \mid w = (w_0, w_1, \ldots, w_M)\}$, $\forall w, z \in \mathscr{S}_h$, we define the inner product and norm as follows

$$
(w, z) = h\sum_{i=1}^{M-1} w_i z_i, \quad \|w\| = \sqrt{(w, w)}, \quad \|w\|_\infty = \max_{0\leq i\leq M}|w_i|, \quad (\delta_x w, \delta_x z)_* = h\sum_{i=1}^{M} \delta_x w_{i-\frac{1}{2}} \delta_x z_{i-\frac{1}{2}},
$$

$$
|w|_1 = (\delta_x w, \delta_x w]^{\frac{1}{2}}, \quad \|w\|_1 = \sqrt{\left(\|w\|^2 + |w|_1^2\right)}.
$$

Through straightforward computations, it can be demonstrated that the following holds,

$$
(\delta_x^2 w, z) = -(\delta_x w, \delta_x z)_*, \qquad \|\delta_x^2 w\| \leq \frac{2|w|_1}{h}, \qquad |w|_1 \leq \frac{2\|w\|}{h}. \tag{14}
$$

The discrete inner product and associated norm are defined as follows:

$$\langle w, z\rangle = \left(\mathscr{S}_x w, -\delta_x^2 z\right) = (\delta_x w, \delta_x z)_* - \frac{h^2}{12}\left(\delta_x^2 w, \delta_x^2 z\right), \qquad \|w\|_* = \sqrt{\langle w, w\rangle}.$$

The following fundamental results can be formally established.
Lemma 5 (see [35]) $\forall\, w \in \mathscr{S}_h$, we obtain

$$\|\mathscr{S}_x w\|^2 \le \|w\|^2 \le \frac{3L^2}{16}\|w\|_*^2, \qquad \|w\|_\infty^2 \le \frac{3L}{8}\|w\|_*^2, \qquad \|w\|_1^2 \le \frac{3(8+L^2)}{16}\|w\|_*^2.$$

Lemma 6 (see [36]) $\forall w \in \mathscr{S}_h$, we obtain

$$\|w\| \le \frac{L^2}{8}\|\delta_x^2 w\|, \qquad \|w\|_*^2 \le \frac{3L^2}{16}\|\delta_x^2 w\|^2. \tag{15}$$

Lemma 7 $\forall w \in \mathscr{S}_h$, the subsequent relation necessarily holds:

$$\left(\sum_{k=1}^{n}\Upsilon_k^n \mathscr{S}_x\left(w^k - w^{k-1}\right), -\delta_x^2 w^{n,\frac{\alpha}{2}}\right) \ge \frac{1}{2}\sum_{k=1}^{n}\Upsilon_k^n\left(\left\|w^k\right\|_*^2 - \left\|w^{k-1}\right\|_*^2\right), \quad 1 \le n \le N. \tag{16}$$

Proof. From the definition of the inner product $\langle\cdot,\cdot\rangle$, we have

$$\left(\sum_{k=1}^{n}\Upsilon_k^n \mathscr{S}_x\left(w^k - w^{k-1}\right), -\delta_x^2 w^{n,\frac{\alpha}{2}}\right) = \left\langle\sum_{k=1}^{n}\Upsilon_k^n\left(w^k - w^{k-1}\right), w^{n,\frac{\alpha}{2}}\right\rangle.$$

By the Corollary 1 of [15] yields

$$\left\langle\sum_{k=1}^{n}\Upsilon_k^n\left(w^k - w^{k-1}\right), w^{n,\frac{\alpha}{2}}\right\rangle \ge \frac{1}{2}\sum_{k=1}^{n}\Upsilon_k^n\left(\left\|w^k\right\|_*^2 - \left\|w^{k-1}\right\|_*^2\right). \tag{17}$$

This proves (16). □

Lemma 8 [38] Suppose nonnegative sequence $\{k_n\}$, $\{s_n\}$ and $\{\rho_n\}$ satisfies

$$\rho_0 \le g_0, \quad \rho_n \le g_0 + \sum_{l=0}^{n-1} s_l + \sum_{l=0}^{n-1} k_l\rho_l, \quad n \ge 1.$$

Then we have

$$\rho_n \le \left(g_0 + \sum_{l=0}^{n-1} s_l\right)\exp\left(\sum_{l=0}^{n-1} k_l\right).$$

Lemma 9 [34] For Υ_k^{n+1} define in (10) and a sufficiently small ε satisfies

$$\Upsilon_n^{n+1} > \Upsilon_{n-1}^{n+1} > \cdots > \Upsilon_0^{n+1} \geq C^F > 0, \tag{18}$$

$$(2\sigma-1)\Upsilon_n^{n+1} - \sigma\Upsilon_{n-1}^{n+1} \geq 0, \tag{19}$$

where $\Upsilon_{-1}^{n+1} = 0$, and C^F is a positive constant.

The preceding lemmas enable rigorous stability analysis and convergence proof for the compact difference scheme (13).

Theorem 1 Consider the numerical solution vector $u^n = (u_0^n,\ u_1^n,\ \ldots,\ u_M^n)$ generated by scheme (13), satisfying homogeneous Dirichlet boundary conditions $u_0^n = u_M^n = 0$. Then when $\|q\|_\infty^2 \leq \frac{32(2\varepsilon-1)}{\varepsilon L^4}$ $\left(\varepsilon > \frac{1}{2}\right)$, we have

$$\|u^n\|_*^2 \leq \left\|u^0\right\|_*^2 + 4\varepsilon\Gamma(1-\alpha)T^\alpha \max_{1\leq n\leq N} \left\|\mathscr{S}_x g^{n-\frac{\alpha}{2}}\right\|^2, \quad 1 \leq n \leq N. \tag{20}$$

Proof. Projecting the governing equation (13) onto $-\delta_x^2 u^{n,\frac{\alpha}{2}}$ through inner product manipulation yields

$$\frac{1}{\mu}\left(\sum_{k=1}^{n}\Upsilon_k^n \mathscr{S}_x\left(u^k - u^{k-1}\right),\, -\delta_x^2 u^{n,\frac{\alpha}{2}}\right)$$

$$= -\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2 - \left(\mathscr{S}_x\left(qu^{n,\frac{\alpha}{2}}\right),\, \delta_x^2 u^{n,\frac{\alpha}{2}}\right) - \left(\mathscr{S}_x g^{n-\frac{\alpha}{2}},\, \delta_x^2 u^{n,\frac{\alpha}{2}}\right), \quad n \in [1,\, n].$$

By Lemma 7, we obtain

$$\frac{1}{2\mu}\sum_{k=1}^{n}\Upsilon_k^n\left(\left\|u^k\right\|_*^2 - \left\|u^{k-1}\right\|_*^2\right)$$

$$\leq -\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2 - \left(\mathscr{S}_x\left(qu^{n,\frac{\alpha}{2}}\right),\, \delta_x^2 u^{n,\frac{\alpha}{2}}\right) - \left(\mathscr{S}_x g^{n-\frac{\alpha}{2}},\, \delta_x^2 u^{n,\frac{\alpha}{2}}\right). \tag{21}$$

When $\|q\|_\infty^2 \leq \frac{32(2\varepsilon-1)}{\varepsilon L^4}$ $\left(\varepsilon > \frac{1}{2}\right)$, we obtain

$$-\left(\mathscr{S}_x\left(qu^{n,\frac{\alpha}{2}}\right),\, \delta_x^2 u^{n,\frac{\alpha}{2}}\right) \leq \frac{\varepsilon\|q\|_\infty^2}{(2\varepsilon-1)}\left\|u^{n,\frac{\alpha}{2}}\right\|^2 + \frac{(2\varepsilon-1)}{4\varepsilon}\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2 \leq \left(1-\frac{1}{4\varepsilon}\right)\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2. \tag{22}$$

From Lemma 6, we have

$$-\left(\mathscr{S}_x\left(qu^{n,\frac{\alpha}{2}}\right),\, \delta_x^2 u^{n,\frac{\alpha}{2}}\right) = q\left\|u^{n,\frac{\alpha}{2}}\right\|_*^2 \leq \left(1-\frac{1}{4\varepsilon}\right)\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2. \tag{23}$$

Thus, the condition $\|q\|_\infty^2 \le \dfrac{32(2\varepsilon-1)}{\varepsilon L^4}$ implies

$$-\left(\mathscr{S}_x\left(qu^{n,\frac{\alpha}{2}}\right), \delta_x^2 u^{n,\frac{\alpha}{2}}\right) \le \left(1-\frac{1}{4\varepsilon}\right)\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2. \tag{24}$$

Combining (24) and the Cauchy-Schwarz inequality,

$$-\left\|\delta_x^2 u^{n,\frac{\alpha}{2}}\right\|^2 - \left(\mathscr{S}_x\left(qu^{n,\frac{\alpha}{2}}\right), \delta_x^2 u^{n,\frac{\alpha}{2}}\right) - \left(\mathscr{S}_x g^{n-\frac{\alpha}{2}}, \delta_x^2 u^{n,\frac{\alpha}{2}}\right) \le \varepsilon \left\|\mathscr{S}_x g^{n-\frac{\alpha}{2}}\right\|^2. \tag{25}$$

Substituting (25) into (21) yields

$$\sum_{k=1}^{n} \Upsilon_k^n \left(\left\|u^k\right\|_*^2 - \left\|u^{k-1}\right\|_*^2\right) \le 2\varepsilon\mu \left\|\mathscr{S}_x g^{n-\frac{\alpha}{2}}\right\|^2, \tag{26}$$

or equivalently

$$\Upsilon_0^n \|u^n\|_*^2 \le \sum_{k=1}^{n-1}\left(\Upsilon_{n-k-1}^n - \Upsilon_{n-k}^n\right)\left\|u^k\right\|_*^2 + \Upsilon_{n-1}^n \left\|u^0\right\|_*^2 + 2\varepsilon\mu\left\|\mathscr{S}_x g^{n-\frac{\alpha}{2}}\right\|^2. \tag{27}$$

Thus we have

$$\Upsilon_0^n \|u^n\|_*^2 \le \sum_{k=1}^{n-1}\left(\Upsilon_{n-k-1}^n - \Upsilon_{n-k}^n\right)\left\|u^k\right\|_*^2 + \Upsilon_{n-1}^n \left(\left\|u^0\right\|_*^2 + 4\varepsilon\Gamma(1-\alpha)T^\alpha\left\|\mathscr{S}_x g^{n-\frac{\alpha}{2}}\right\|^2\right). \tag{28}$$

Recursive application of identity (28) through mathematical induction establishes the target inequality (20). □
Define

$$C_3 = \sqrt{\left(4T^\alpha L\Gamma(1-\alpha)C_F^2\right)}.$$

From Theorem 1 and Lemma 4, we can obtain the following theorem.
Theorem 2 Suppose the conditions in Theorems 1 is satisfied. Then we obtain

$$\|W^n - w^n\| \le \frac{C_3 L\sqrt{3\varepsilon}}{4}\left(\tau^2 + h^4 + \varepsilon\right), \qquad 1 \le n \le N, \tag{29}$$

$$\|W^n - w^n\|_1 \le \frac{C_3\sqrt{3(8+L^2)\varepsilon}}{4}\left(\tau^2 + h^4 + \varepsilon\right), \qquad 1 \le n \le N, \tag{30}$$

$$\|W^n - w^n\|_\infty \le \frac{C_3\sqrt{6L\varepsilon}}{4}\left(\tau^2 + h^4 + \varepsilon\right), \qquad 1 \le n \le N. \tag{31}$$

5. Numerical validation and discussion results

We now validate our fast $FL2-1_{\delta}$ scheme against the direct $L2-1_{\delta}$ scheme using two examples. The norm errors are defined as:

$$\mathrm{E}(\tau, h)=\max_{0\leq n\leq N}\|w(x_i, t_n)^n-w_i^n\|, \quad \mathrm{O}^{\mathrm{t}}(\tau, h)=\log_2\left(\frac{\mathrm{E}(2\tau, h)}{\mathrm{E}(\tau, h)}\right), \quad \mathrm{O}^{\mathrm{s}}(\tau, h)=\log_2\left(\frac{\mathrm{E}(\tau, 2h)}{\mathrm{E}(\tau, h)}\right). \tag{32}$$

Example 1 When $x\in[0, 1]$, $t\in[0, 1]$, we consider the problem (4), $\psi_0(t)=0$, $\psi_L(t)=1+t^{3+\alpha}$, $\phi(x)=2x-x^2$ and

$$f=4(1+x)^{-1}\left(1+t^{3+\alpha}\right)+\frac{2x-x^2}{6}\left(\Gamma(4+\alpha)t^3-6(1+t^{3+\alpha})(1+2x)^2\right), \tag{33}$$

$$\beta_1(x)=(1+x)^{-1}, \qquad \beta_2(x)=4x^2+4x+1, \tag{34}$$

$$\rho(x)=(1+2x)^2-3/(4(1+x)^2). \tag{35}$$

We first solve the problem numerically using the compact difference scheme (13), then using scheme (2.18) from [37]. Table 1 lists $\mathrm{E}(\tau, h)$ and $\mathrm{O}^{\mathrm{t}}(\tau, h)$, confirming comparable accuracy for both schemes. With spatial refinement from $h=1/4$ to $1/64$ and fixed $\tau=1/15{,}000$, Table 2 demonstrates optimal $O(h^4)$ convergence for both methods.

Figure 1a displays $T=1$ errors for the $FL2-1_{\delta}$ scheme under varying h and τ, the results confirm that both schemes exhibit comparable accuracy. Figure 1b compares CPU times versus N, and demonstrates that $FL2-1_{\delta}$ has near-linear complexity and significantly faster performance than the $L2-1_{\delta}$ scheme in [31] (cited in [37]).

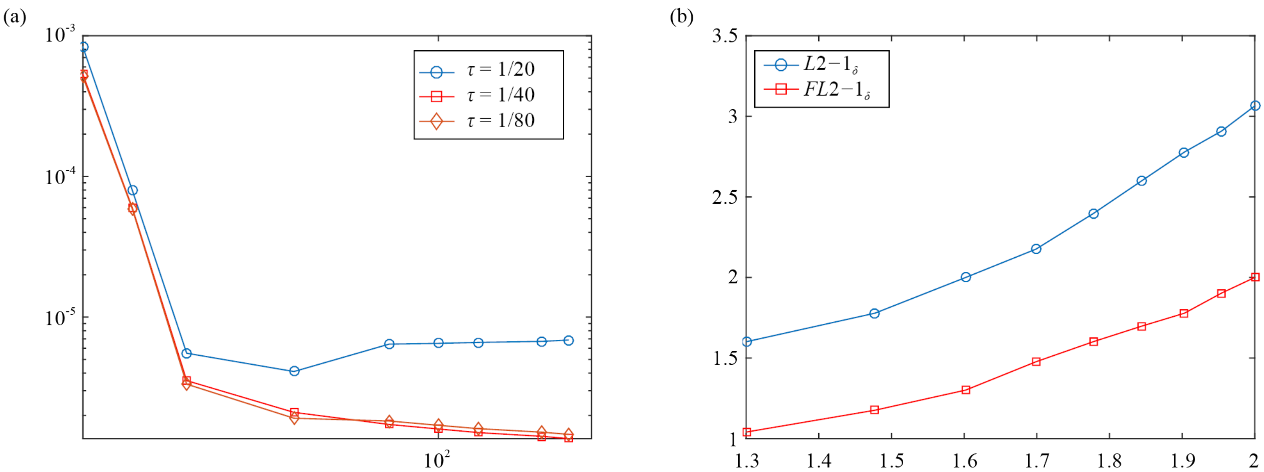

Figure 1. (a): Error when $T=1$ for different h_x, h_y and different τ; (b): CPU time when $\alpha=1/2$, $T=1$

Table 1. The $E(\tau, h)$ and $O^t(\tau, h)$ for Example 1 ($h = 1/200$)

α	τ	$L2-1_\delta$ in [37]		$FL2-1_\delta$	
		$E(\tau, h)$	$O^t(\tau, h)$	$E(\tau, h)$	$O^t(\tau, h)$
1/4	1/20	9.9166e-05		1.7367e-04	
	1/40	2.5350e-05	1.9678	4.4337e-05	1.9698
	1/80	6.4247e-06	1.9803	1.1227e-05	1.9816
	1/160	1.6197e-06	1.9879	2.8285e-06	1.9888
	1/320	4.0702e-07	1.9925	7.1051e-07	1.9931
	1/640	1.021e-07	1.9952	1.7817e-07	1.9956
1/2	1/20	1.9124e-04		3.3641e-04	
	1/40	4.9218e-05	1.9581	8.6453e-05	1.9602
	1/80	1.2561e-05	1.9702	2.2037e-05	1.9720
	1/160	3.1870e-06	1.9787	5.5851e-06	1.9803
	1/320	8.0519e-07	1.9845	1.4099e-06	1.9860
	1/640	2.0284e-07	1.9890	3.5492e-07	1.9900
3/4	1/20	2.4746e-04		4.3541e-04	
	1/40	6.3817e-05	1.9552	1.1244e-04	1.9532
	1/80	1.6383e-05	1.9618	2.8882e-05	1.9610
	1/160	4.1896e-06	1.9673	7.3853e-06	1.9674
	1/320	1.0679e-06	1.9721	1.8815e-06	1.9728
	1/640	2.7141e-07	1.9762	4.7794e-07	1.9770

Table 2. The $E(\tau, h)$ and $O^s(\tau, h)$ for Example 1 ($\tau = 1/15{,}000$)

α	h	$L2-1_\delta$ in [37]		$FL2-1_\delta$	
		$E(\tau, h)$	$O^s(\tau, h)$	$E(\tau, h)$	$O^s(\tau, h)$
1/4	1/4	3.1665e-04		4.2478e-04	
	1/8	2.0867e-05	3.9236	2.7838e-05	3.9316
	1/16	1.3219e-06	3.9805	1.7842e-06	3.9637
	1/32	8.3002e-08	3.9933	1.1197e-07	3.9941
	1/64	5.2996e-09	3.9692	7.1046e-09	3.9782
1/2	1/4	3.1094e-04		4.1668e-04	
	1/8	2.0492e-05	3.9235	2.7306e-05	3.9317
	1/16	1.2983e-06	3.9804	1.7519e-06	3.9622
	1/32	8.1624e-08	3.9915	1.1003e-07	3.9930
	1/64	5.3214e-09	3.9391	7.0980e-09	3.9543
3/4	1/4	3.0345e-04		4.0606e-04	
	1/8	2.0001e-05	3.9233	2.6639e-05	3.9301
	1/16	1.2672e-06	3.9803	1.7094e-06	3.9620
	1/32	7.9734e-08	3.9903	1.0739e-07	3.9925
	1/64	5.2707e-09	3.9191	7.0057e-09	3.9382

Example 2 In this example, in the domain [0, 1] × [0, 1], let $\beta_1 = 1/(1+x+t)$, $\beta_2 = (x+t)^2$ and

$$f = \frac{1}{6e^x}\Gamma(4+\alpha)t^3 - (1+t^{3+\alpha})\left(\frac{2+x+t}{1+x+t} + (x+t)^2\right)\mathrm{e}^{-x}, \tag{36}$$

$$\rho = (x+t)^2 - 3/(4(1+x+t)^2). \tag{37}$$

Tables 3 and Table 4 present $\mathrm{E}(\tau, h)$, $\mathrm{O}^{\mathrm{t}}(\tau, h)$, and $\mathrm{O}^{\mathrm{s}}(\tau, h)$ for $\alpha = 1/4, 1/2, 3/4$. Numerical results confirm the theoretical rates: second-order temporal convergence and fourth-order spatial convergence are consistently achieved.

Figure 2a displays $T = 1$ errors under h-τ variations for $FL2-1_\delta$, confirming unconditional stability. The Figure 2b demonstrates significantly faster computation versus the $L2-1_\delta$ scheme.

Table 3. The $\mathrm{E}(\tau, h)$ and $\mathrm{O}^{\mathrm{t}}(\tau, h)$ for Example 2 ($h = 1/200$)

		$L2-1_\delta$ in [37]		$FL2-1_\delta$	
α	τ	$\mathrm{E}(\tau, h)$	$\mathrm{O}^{\mathrm{t}}(\tau, h)$	$\mathrm{E}(\tau, h)$	$\mathrm{O}^{\mathrm{t}}(\tau, h)$
1/4	1/20	2.1181e-04		2.9146e-04	
	1/40	5.3717e-05	1.9793	7.3918e-05	1.9793
	1/80	1.3539e-05	1.9883	1.8630e-05	1.9883
	1/160	3.4007e-06	1.9932	4.6795e-06	1.9932
	1/320	8.5251e-07	1.9960	1.1731e-06	1.9961
	1/640	2.1347e-07	1.9977	2.9373e-07	1.9977
1/2	1/20	4.0835e-04		5.6123e-04	
	1/40	1.0388e-04	1.9749	1.4276e-04	1.9750
	1/80	2.6261e-05	1.9839	3.6090e-05	1.9839
	1/160	6.6145e-06	1.9892	9.0899e-06	1.9892
	1/320	1.6621e-06	1.9926	2.2841e-06	1.9926
	1/640	4.1700e-07	1.9949	5.7305e-07	1.9949
3/4	1/20	5.3722e-04		7.3699e-04	
	1/40	1.3688e-04	1.9726	1.8777e-04	1.9727
	1/80	3.4717e-05	1.9791	4.7624e-05	1.9792
	1/160	8.7810e-06	1.9832	1.2045e-05	1.9832
	1/320	2.2164e-06	1.9862	3.0402e-06	1.9862
	1/640	5.5854e-07	1.9885	7.6611e-07	1.9885

Table 4. The $E(\tau, h)$ and $O^s(\tau, h)$ for Example 2 ($\tau = 1/20{,}000$)

α	h	$L2-1_\delta$ in [37]		$FL2-1_\delta$	
		$E(\tau, h)$	$O^s(\tau, h)$	$E(\tau, h)$	$O^s(\tau, h)$
1/4	1/4	8.1464e-05		1.0890e-04	
	1/8	5.3901e-06	3.9178	7.4506e-06	3.8695
	1/16	3.4150e-07	3.9803	4.7205e-07	3.9803
	1/32	2.1407e-08	3.9957	2.9706e-08	3.9901
	1/64	1.3306e-09	4.0079	1.8461e-09	4.0082
1/2	1/4	7.0876e-05		9.5630e-05	
	1/8	4.6814e-06	3.9203	6.4827e-06	3.8828
	1/16	2.9644e-07	3.9811	4.1187e-07	3.9763
	1/32	1.8574e-08	3.9964	2.5861e-08	3.9933
	1/64	1.1485e-09	4.0155	1.5988e-09	4.0158
3/4	1/4	6.4563e-05		8.6429e-05	
	1/8	4.2517e-06	3.9246	5.8977e-06	3.8733
	1/16	2.6904e-07	3.9822	3.7298e-07	3.9829
	1/32	1.6851e-08	3.9969	2.3455e-08	3.9911
	1/64	1.0384e-09	4.0204	1.4451e-09	4.0206

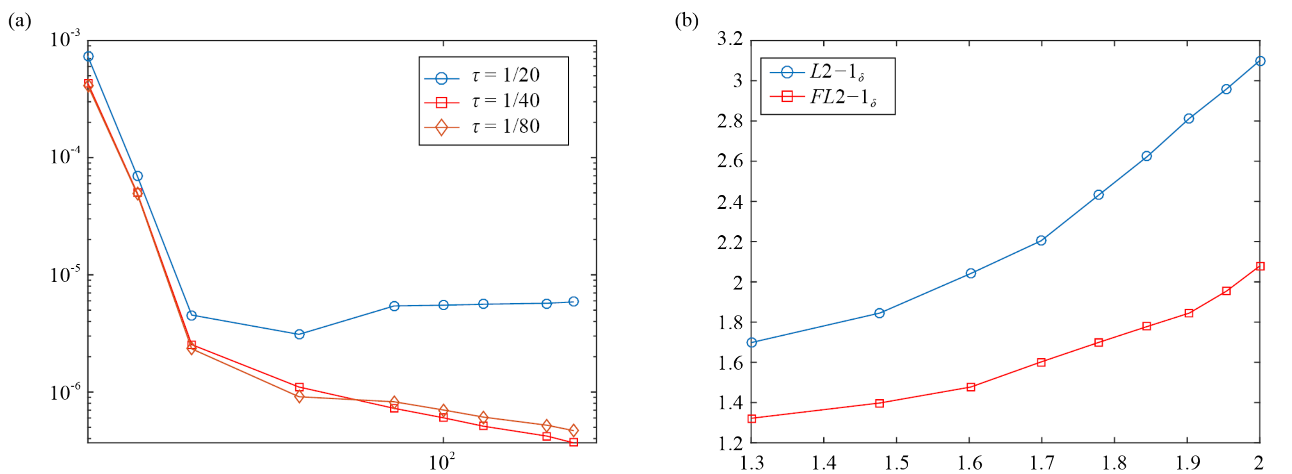

Figure 2. (a): Error when $T = 1$ for different h_x, h_y; (b): CPU time when $\alpha = 1/2$, $T = 1$

6. Concluding remarks

We develop a high-order compact finite difference scheme for TFCRD equations with variable coefficients. The method integrates the $FL2$-1_σ formula (Liouville-Caputo derivative) with fourth-order compact spatial discretization. Rigorous analysis proves unique solvability, unconditional stability, and $\mathscr{O}(\tau^2 + h^4)$ convergence in L^2-norm, with accuracy independent of the fractional order α. This reduces computational cost by orders of magnitude compared to [37]. Numerical tests validate theoretical results and demonstrate computational superiority.

Data availability statement

The datasets used and/or analysed during the current study available from the corresponding author on reasonable request.

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Author's contributions

Lei Ren: Writing-review and editing, Conceptualization, Methodology, Project administration; Shixin Jin: Funding, Conceptualization, Methodology.

Conflict of interest

The authors declare no competing financial interest.

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