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A second-order difference scheme for the time fractional substantial diffusion equation

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ABSTRACT

In this work, a second-order approximation of the fractional substantial derivative is presented by considering a modified shifted substantial Grünwald formula and its asymptotic expansion. Moreover, the proposed approximation is applied to a fractional diffusion equation with fractional substantial derivative in time. With the use of the fourth-order compact scheme in space, we give a fully discrete Grünwald–Letnikov-formula-based compact difference scheme and prove its stability and convergence by the energy method under smooth assumptions. In addition, the problem with nonsmooth solution is also discussed, and an improved algorithm is proposed to deal with the singularity of the fractional substantial derivative. Numerical examples show the reliability and efficiency of the scheme.

1. Introduction

Anomalous sub-diffusion process, commonly described by the continuous time random walks (CTRWs), and also known as non-Brownian sub-diffusion, arises in numerous physical, chemical and biological systems; see [1–4]. The Feynman–Kac formula named after Richard Feynman and Mark Kac, establishes a link between parabolic partial differential equations (PDEs) and Brownian functionals. To figure out the probability density function (PDF) of some non-Brownian functionals, the fractional Feynman–Kac equation has been derived in [5–9]. The non-Brownian functionals can be defined by $A = \int_0^t U(x(\tau))\mathrm{d}\tau$, where $x(t)$ is the trajectory of a non-Brownian particle and different choices of $U(x)$ can depict diverse systems. In particular, if taking $U(x) \equiv 0$, the fractional Feynman–Kac equation reduces to the well-known fractional Fokker–Planck equation; see [5,6,10] for details. Lévy walks give a proper dynamical description in the superdiffusive domain, where the temporal and spatial variables of Lévy walks are strongly correlated and the PDFs of waiting time and jump length are spatiotemporal coupling [8]. Thus, an important operator, fractional substantial derivative has been proposed to describe the CTRW models with coupling PDFs. This spatiotemporal coupling operator was also presented in [7], where the CTRW model with position-velocity coupling PDF was discussed. Recently, Carmi and Barkai [5] also used the substantial derivative to derive the forward and backward fractional Feynman–Kac equations. Due to its potential properties

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and wide application, the fractional substantial derivative has attracted many scholars' attention; see [11,12] and references therein.

The fractional substantial derivative operator of order α $(n-1<\alpha<n)$ is defined by [12]

$$ {}_aD_t^{\alpha,\lambda}f(t) = {}_aD_t^{n,\lambda}[{}_aI_t^{n-\alpha,\lambda}f](t), \qquad {}_aI_t^{\alpha,\lambda}f(t) = \frac{1}{\Gamma(\alpha)}\int_a^t \frac{f(\xi)}{(t-\xi)^{1-\alpha}e^{\lambda(t-\xi)}}d\xi; \tag{1.1} $$

where $\alpha>0$, λ is a constant or a function independent of variable t, ${}_aI_t^{\alpha,\lambda}$ denotes the fractional substantial operator, and

$$ {}_aD_t^{n,\lambda} = \left(\frac{d}{dt}+\lambda\right)^n = \left(\frac{d}{dt}+\lambda\right)\left(\frac{d}{dt}+\lambda\right)\cdots\left(\frac{d}{dt}+\lambda\right). $$

It is noted that if λ is a nonnegative constant, then the fractional substantial derivative is equivalent to the Riemann–Liouville tempered derivative defined in [13–15], and taking $\lambda=0$ in (1.1) leads to the left Riemann–Liouville derivative. Meanwhile, to obtain the non-Brownian functionals, whose path integrals are over Lévy trajectories, the space-fractional Fokker–Planck equation and the tempered space fractional diffusion equations have been widely used; see [16–18].

The current work is devoted to proposing a second-order Grünwald–Letnikov-formula-based approximation for the fractional substantial derivative (1.1), and applying it to derive a high-order fully discrete scheme for the time fractional substantial diffusion equation (TFSDE)

$$ {}_0D_t^{\alpha,\lambda}u(\mathbf{x},t) = \Delta u(\mathbf{x},t) + F(\mathbf{x},t), \quad \mathbf{x}\in\Omega,\ t\in(0,T], \tag{1.2} $$

$$ u(\mathbf{x},0) = u_0(\mathbf{x}), \quad \mathbf{x}\in\Omega, \tag{1.3} $$

$$ u(\mathbf{x},t)|_{\mathbf{x}\in\partial\Omega} = \phi(\mathbf{x},t), \quad t\in(0,T], \tag{1.4} $$

where Δ is the Laplacian operator, $\mathbf{x}$ denotes the one-dimensional or two-dimensional space variable, $\partial\Omega$ is the boundary of domain Ω, $F(\mathbf{x},t)$, $u_0(\mathbf{x})$ and $\phi(\mathbf{x},t)$ are given functions; ${}_0D_t^{\alpha,\lambda}$ is the substantial derivative defined by (1.1), and $0<\alpha\le 1$.

The main novelty of our paper is the derivation of a second-order operator, which is based on the modified definition of the Grünwald derivative (see Section 3.4, [19]), for the approximation of the fractional substantial derivative. The modified Grünwald derivative is defined by [19]

$$ {}_0^{GL}D_t^{\alpha}f(t) \equiv \lim_{\tau\to 0}\frac{1}{\tau^\alpha}\sum_{k=0}^{[t/\tau]} g_k^\alpha f\left(t-k\tau+\frac{\alpha}{2}\tau\right), \quad g_k^\alpha = (-1)^k\binom{\alpha}{k}. \tag{1.5} $$

Actually, if dropping the term $\frac{\alpha}{2}\tau$ off in the right side of above definition, one gets the original definition of the Grünwald derivative. The advantage of the modified Grünwald derivative is that it permits the design of more efficient algorithms to approximate the Riemann–Liouville fractional derivatives than using the shifted Grünwald–Letnikov formula directly. In this paper, by developing the modified Grünwald derivative and the shifted Grünwald–Letnikov formula to the fractional substantial derivative, a modified shifted substantial Grünwald formula and its asymptotic expansion are presented. Based upon the asymptotic expansion, a second-order approximation of the fractional substantial derivative is derived.

There are also some other approaches for the approximation of fractional derivatives, such as the $L1$ approximation [20,21], the fractional linear multi-step methods (FLMMs) developed by Lubich [22], the $L2$ approximation with using superior convergence [23,24], etc. However, to the best of authors' knowledge, very limited work has been presented for the fractional substantial derivative. Chen and Deng [12] extended the p-th order FLMMs [25] to approximate the fractional substantial derivative, and applied it to solve the fractional Feynman–kac equation [26] lately. Very recently, Chen and Deng [27] proposed some algorithms for the equation with the fractional substantial derivative in time and the tempered fractional derivatives in space, in which the numerical stability and error estimate have been given for a scheme with the first-order accuracy in time and the second-order accuracy in space.

The main goal of our paper is to construct a second-order approximation for the time fractional substantial derivative, and subsequently to solve the TFSDE (1.2)–(1.4) by combining the existed fourth-order compact approximation for the space derivatives [28], and establish the numerical stability and error estimate of the derived fully discretized scheme.

In this work, we assume that the solution to the underlying equation satisfies suitable regularity requirements. The assumption can be satisfied in certain conditions, while it may not hold for many time-fractional differential equations; see related discussion for the case $\lambda=0$ in [29–32]. To circumvent the requirement of high regularity of the solution, we apply starting quadrature to add correction terms in the proposed scheme. The starting quadrature was first developed in [25], and has been used to deal with problems with nonsmooth solution; see [26,22]. The validity of the proposed algorithm is illustrated in Example 6.3 by solving a two-dimensional time fractional substantial diffusion equation.

The remainder of this paper is organized as follows. In Section 2, a second-order operator for the approximation of the fractional substantial derivative is derived. In Section 3, the proposed approximation is applied to TFSDE (1.2)–(1.4), and a fully discretized scheme is derived by combining the fourth-order compact formula in space. In Section 4, we give a discrete prior estimate for the numerical solution, and then prove the convergence and stability of the proposed scheme. The behavior of our proposed scheme when applied to solve problems with non-smooth solution is further discussed and the improved algorithm is proposed in Section 5. Numerical results are presented in Section 6. Some concluding remarks are included in the final section.

2. A second-order approximation for the fractional substantial derivative

In this section, we first present a second-order approximation for the fractional substantial derivative. For $0 < \alpha \leq 1$, we give the following identities from (1.1):

$$ {}_aI_t^{\alpha,\lambda} f(t) = e^{-\lambda t} {}_aI_t^{\alpha}[e^{\lambda t} f(t)], \qquad {}_aD_t^{\alpha,\lambda} f(t) = e^{-\lambda t} {}_aD_t^{\alpha}[e^{\lambda t} f(t)]. \tag{2.1} $$

Moreover, if $f(a) = 0$, by the composition formula [33], it holds that

$$ {}_aI_t^{\alpha,\lambda} {}_aD_t^{\alpha,\lambda} f(t) = f(t). \tag{2.2} $$

Based on the definition of the modified Grünwald derivative [19] and the shifted Grünwald–Letnikov formula [34], we define

$$ A_{\tau,r}^{\alpha,\lambda} f(t) = \frac{1}{\tau^\alpha} \sum_{k=0}^{+\infty} e^{-\lambda(k-r)\tau} g_k^\alpha f(t-(k-r)\tau), \quad \forall\, \alpha > 0 \tag{2.3} $$

where τ is the step size, and $\{g_k^\alpha\}$ are the coefficients of the power series expansion of the function $(1-z)^\alpha$, i.e.,

$$ (1-z)^\alpha = \sum_{k=0}^{+\infty} (-1)^k \binom{\alpha}{k} z^k = \sum_{k=0}^{+\infty} g_k^\alpha z^k, \quad \forall\, |z| < 1. \tag{2.4} $$

Obviously, $g_k^\alpha = (-1)^k \binom{\alpha}{k}$ can also be evaluated recursively by

$$ g_0^\alpha = 1, \quad g_k^\alpha = \left(1 - \frac{\alpha+1}{k}\right) g_{k-1}^\alpha, \quad k = 1, 2, \ldots. \tag{2.5} $$

Let $f \in L_1(\mathbb{R})$. Define the function space $\mathscr{C}^{n+\alpha}(\mathbb{R})$ by

$$ \mathscr{C}^{n+\alpha}(\mathbb{R}) = \left\{ f \,\Big|\, \int_{-\infty}^{+\infty} (1+|\omega|)^{n+\alpha} |\hat{f}(\omega)| d\omega < \infty \right\}, $$

where $\hat{f}(\omega) = \int_{-\infty}^{+\infty} e^{i\omega t} f(t) dt$ is the Fourier transform of $f(t)$.

Motivated by the work in [34], we present an asymptotic expansion of $A_{\tau,r}^{\alpha,\lambda} f(t)$.

Lemma 2.1. *Suppose that $f \in L_1(\mathbb{R})$ and $f \in \mathscr{C}^{n+\alpha}(\mathbb{R})$. Then*

$$ A_{\tau,r}^{\alpha,\lambda} f(t) = {}_{-\infty}D_t^{\alpha,\lambda} f(t) + \sum_{k=1}^{n-1} c_{r,k}^\alpha \, {}_{-\infty}D_t^{\alpha+k,\lambda} f(t) \tau^k + \mathcal{O}(\tau^n) \tag{2.6} $$

uniformly holds in $t \in \mathbb{R}$ as $\tau \to 0$, where $c_{r,k}^\alpha$ are the coefficients of the power series expansion of the function $W_{\alpha,r}(z) = (\frac{1-e^{-z}}{z})^\alpha e^{rz}$.

Proof. Using the Fourier transform, we obtain

$$ \begin{aligned} \mathcal{F}(A_{\tau,r}^{\alpha,\lambda} f)(\omega) &= \frac{1}{\tau^\alpha} \sum_{k=0}^{\infty} e^{-\lambda(k-r)\tau} g_k^\alpha \mathcal{F}(f(t-(k-r)\tau))(\omega) \\ &= \frac{1}{\tau^\alpha} \sum_{k=0}^{\infty} e^{-\lambda(k-r)\tau} g_k^\alpha e^{i\omega(k-r)\tau} \hat{f}(\omega) \\ &= \frac{1}{\tau^\alpha} (1 - e^{-(\lambda - i\omega)\tau})^\alpha e^{r(\lambda-i\omega)\tau} \hat{f}(\omega) \\ &= (\lambda - i\omega)^\alpha \left(\frac{1 - e^{-(\lambda-i\omega)\tau}}{(\lambda - i\omega)\tau} \right)^\alpha e^{r(\lambda-i\omega)\tau} \hat{f}(\omega) \\ &= (\lambda - i\omega)^\alpha W_{\alpha,r}((\lambda - i\omega)\tau) \hat{f}(\omega). \end{aligned} $$

Observe that $c_{r,0}^\alpha = 1$ and

$$ \mathcal{F}({}_{-\infty}D_t^{\alpha+k,\lambda} f)(\omega) = (\lambda - i\omega)^{\alpha+k} \hat{f}(\omega) $$

for $k = 0, 1, 2 \cdots$. Therefore, there exists

$$ \mathcal{F}(A_{\tau,r}^{\alpha,\lambda} f)(\omega) = \sum_{k=0}^{n-1} c_{r,k}^\alpha \mathcal{F}({}_{-\infty}D_t^{\alpha+k,\lambda} f)(\omega) \tau^k + \Phi(\omega, \tau), \tag{2.7} $$

where

$$\Phi(\omega,\tau)=(\lambda-i\omega)^{\alpha}\left[W_{\alpha,r}((\lambda-i\omega)\tau)-\sum_{k=0}^{n-1}c_{r,k}^{\alpha}(\lambda-i\omega)^{k}\tau^{k}\right]\hat{f}(\omega).$$

Taking inverse Fourier transform on the both sides of (2.7) leads to

$$A_{\tau,r}^{\alpha,\lambda}f(t)-\sum_{k=0}^{n-1}c_{r,k}^{\alpha}\,{}_{-\infty}D_t^{\alpha+k,\lambda}f(t)\tau^{k}=\frac{1}{2\pi}\int_{-\infty}^{+\infty}\Phi(\omega,\tau)e^{-i\omega t}d\omega. \tag{2.8}$$

Due to the fact that $f\in\mathscr{C}^{n+\alpha}(\mathbb{R})$ and $W_{\alpha,r}(z)=\sum_{k=0}^{n-1}c_{r,k}^{\alpha}z^{k}+O(z^{n})$, then there exists a constant c such that

$$\begin{aligned}&A_{\tau,r}^{\alpha,\lambda}f(t)-{}_{-\infty}D_t^{\alpha,\lambda}f(t)-\sum_{k=1}^{n-1}c_{r,k}^{\alpha}\,{}_{-\infty}D_t^{\alpha+k,\lambda}f(t)\tau^{k}\\&\quad\le\frac{1}{2\pi}\int_{-\infty}^{+\infty}|\Phi(\omega,\tau)|d\omega\le c\int_{-\infty}^{+\infty}(1+|\omega|)^{n+\alpha}|\hat{f}(\omega)|d\omega\cdot\tau^{n}=\mathcal{O}(\tau^{n}).\end{aligned}$$

for sufficiently small τ. This ends the proof. □

Remark 2.2. Take $\lambda=0,\ \alpha=1$ in above lemma. When $r=0$, (2.6) reduces to the backward difference operator for the standard derivative:

$$f'(t)=\frac{f(t)-f(t-\tau)}{\tau}+\mathcal{O}(\tau);$$

when $r=\frac{\alpha}{2}=\frac{1}{2}$, (2.6) reduces to the central difference quotient operator:

$$f'(t)=\frac{f\left(t+\frac{1}{2}\tau\right)-f\left(t-\frac{1}{2}\tau\right)}{\tau}+\mathcal{O}(\tau^{2}).$$

On the other hand, the accuracy can be improved by shifting from the backward difference formula to the central difference counterpart. From this point of view, the fractional shift in the formula (2.6) is natural and reasonable to achieve high accuracy.

From Lemma 2.1, we can take $A_{\tau,r}^{\alpha,\lambda}f(t)$ as a first-order approximation to the fractional substantial derivative ${}_{-\infty}D_t^{\alpha,\lambda}f(t)$, that is,

$$A_{\tau,r}^{\alpha,\lambda}f(t)={}_{-\infty}D_t^{\alpha,\lambda}f(t)+\mathcal{O}(\tau),$$

which is consistent with the approximation of the Riemann–Liouville derivative by the shifted Grünwald–Letnikov formula [34]. Note that $c_{r,1}^{\alpha}=r-\frac{\alpha}{2}$. We take $t=s-r\tau$ and $r=\frac{\alpha}{2}$ in (2.6), then it follows that

$$A_{\tau,r}^{\alpha,\lambda}f\left(s-\frac{\alpha}{2}\tau\right)={}_{-\infty}D_t^{\alpha,\lambda}f\left(s-\frac{\alpha}{2}\tau\right)+\mathcal{O}(\tau^{2}).$$

By (2.3), and using the Lagrange linear interpolation at the points $t=s$ and $t=s-\tau$ for the approximation of ${}_{-\infty}D_t^{\alpha,\lambda}f(s-r\tau)$, and replacing s with t, we can derive the following second-order Grünwald–Letnikov-formula-based approximation for the fractional substantial derivative.

Theorem 2.3. *Suppose that $f\in L_1(\mathbb{R})$ and $f\in\mathscr{C}^{2+\alpha}(\mathbb{R})$. Then*

$$\left(1-\frac{\alpha}{2}\right){}_{-\infty}D_t^{\alpha,\lambda}f(t)+\frac{\alpha}{2}{}_{-\infty}D_t^{\alpha,\lambda}f(t-\tau)=\frac{1}{\tau^{\alpha}}\sum_{k=0}^{+\infty}g_k^{\alpha,\lambda}f(t-k\tau)+\mathcal{O}(\tau^{2})$$

uniformly holds in $t\in\mathbb{R}$ as $\tau\to0$, where $g_k^{\alpha,\lambda}=e^{-(k-\frac{\alpha}{2})\lambda\tau}g_k^{\alpha}$.

To apply Theorem 2.3 to the generic function $f(t)(f(0)=0)$ on $[0,+\infty)$, we make the zero extension as follows:

$$\tilde{f}(t)=\begin{cases}f(t), & t\in[0,+\infty),\\ 0, & \text{others}\end{cases}$$

and further assume that $\tilde{f}(t)$ satisfies the assumptions in Theorem 2.3, i.e., $\tilde{f}(t)\in\mathscr{C}^{2+\alpha}(\mathbb{R})$. Then it follows that

$$\left(1-\frac{\alpha}{2}\right){}_{0}D_t^{\alpha,\lambda}f(t)+\frac{\alpha}{2}{}_{0}D_t^{\alpha,\lambda}f(t-\tau)=\frac{1}{\tau^{\alpha}}\sum_{k=0}^{[\frac{t}{\tau}]}g_k^{\alpha,\lambda}f(t-k\tau)+\mathcal{O}(\tau^{2}). \tag{2.9}$$

3. Derivation of the numerical scheme

In this section, we construct a numerical scheme for the problem (1.2)–(1.4). We first derive a semi-discretized scheme by the proposed approximation (2.9). Subsequently, with the use of the fourth-order compact finite difference approximation of the space derivatives [28], we give a fully discrete scheme. In what follows, we suppose that $u(\mathbf{x},0)=0$ without loss of generality. Otherwise, consider the equation with the solution $v(\mathbf{x},t)=u(\mathbf{x},t)-e^{-\lambda t}u(\mathbf{x},0)$ instead. Furthermore, assume that the extended $u(\cdot,t)\in\mathscr{C}^{2+\alpha}(\mathbb{R})$.

3.1. A semi-discrete scheme

Now we are in the position to discrete (1.2) in time. Take the uniform time step size $\tau=T/N$ and let $t_n=n\tau,\ 0\le n\le N$. The temporal domain $[0,T]$ is covered by $\Omega_\tau=\{t_n\mid 0\le n\le N\}$. For a given grid function $v=\{v^n\}_{n=0}^N$ defined on Ω_τ, we introduce the average operator:

$$\mathscr{A}_t^\alpha v^n=\left(1-\frac{\alpha}{2}\right)v^n+\frac{\alpha}{2}v^{n-1} \tag{3.1}$$

and the discrete difference quotient operator:

$$\delta_t^{\alpha,\lambda}v^n=\frac{1}{\tau^\alpha}\sum_{k=0}^{n}g_k^{\alpha,\lambda}v^{n-k}. \tag{3.2}$$

Considering Eq. (1.2) at the grid points $(\mathbf{x},t_n)$, we have

$${}_0D_t^{\alpha,\lambda}u(\mathbf{x},t_n)=\Delta u(\mathbf{x},t_n)+F(\mathbf{x},t_n),\quad 0\le n\le N. \tag{3.3}$$

Performing the average operator $\mathscr{A}_t^\alpha$ defined in (3.1) on Eq. (3.3), we have

$$\mathscr{A}_t^\alpha\,{}_0D_t^{\alpha,\lambda}u(\mathbf{x},t_n)=\mathscr{A}_t^\alpha\Delta u(\mathbf{x},t_n)+\mathscr{A}_t^\alpha F(\mathbf{x},t_n),\quad 1\le n\le N.$$

Applying the formula (2.9) and combining (3.2) yield

$$\delta_t^{\alpha,\lambda}u(\mathbf{x},t_n)=\mathscr{A}_t^\alpha\Delta u(\mathbf{x},t_n)+\mathscr{A}_t^\alpha F(\mathbf{x},t_n)+\mathcal{O}(\tau^2),\quad 1\le n\le N. \tag{3.4}$$

Noting that (3.4) is a semi-discretization to (1.2), in next subsection, we will derive a full discretization by the finite difference method. It is worth to point out that (3.4) can also be solved by many other methods that we mentioned in the introduction part, such as spectral method, finite element method, discontinuous Galerkin method, etc.

3.2. A fully discrete scheme

In this part, we use the fourth-order compact approximation for the spatial discretization of the problem (1.2)–(1.4). To fix the idea, we consider only one-dimensional problem (1.2)–(1.4) in this subsection and illustrate the generalization to two-dimensional case via an example in Section 6.

Let $\Omega=(a,b)$. Take a positive integer M and let $h=(b-a)/M$, $x_i=ih$, $0\le i\le M$. Then the spatial domain $[a,b]$ is covered by $\Omega_h=\{x_i\mid 0\le i\le M\}$.

For completeness of the paper, we introduce some results that are helpful for understanding the construction of the scheme. The following lemma is required to achieve high-order accuracy for spatial discretization.

Lemma 3.1 ([28]). *Denote $\theta(s)=(1-s)^3[5-3(1-s)^2]$. If $G(x)\in C^6[x_{i-1},x_{i+1}]$, $x_{i+1}=x_i+h$, $x_{i-1}=x_i-h$, it holds that*

$$\begin{aligned}\frac{1}{12}[G''(x_{i-1})+10G''(x_i)+G''(x_{i+1})]&=\frac{G(x_{i-1})-2G(x_i)+G(x_{i+1})}{h^2}\\&\quad+\frac{h^4}{360}\int_0^1[G^{(6)}(x_i-sh)+G^{(6)}(x_i+sh)]\theta(s)ds,\quad 1\le i\le M-1.\end{aligned}$$

Introduce the average operator $\mathscr{A}_x$ in spatial direction as

$$\mathscr{A}_x v_i=\begin{cases}\frac{1}{12}(v_{i-1}+10v_i+v_{i+1}), & 1\le i\le M-1,\\ v_i, & i=0 \text{ or } M.\end{cases}$$

Denote by δ_x^2 the second-order central difference quotient operator, that is

$$\delta_x^2 v_i=\frac{1}{h^2}(v_{i-1}-2v_i+v_{i+1}).$$

Taking $\mathbf{x} = x_i$ and performing the average operator $\mathcal{A}_x$ on both sides of (3.4) gives

$$\mathcal{A}_x \delta_t^{\alpha,\lambda} u(x_i, t_n) = \mathcal{A}_x \mathcal{A}_t^{\alpha} \partial_x^2 u(x_i, t_n) + \mathcal{A}_x \mathcal{A}_t^{\alpha} F(x_i, t_n) + \mathcal{O}(\tau^2), \quad 1 \le i \le M-1,\ 1 \le n \le N. \tag{3.5}$$

Define the grid functions

$$U_i^n = u(x_i, t_n), \qquad F_i^n = F(x_i, t_n), \quad 0 \le i \le M,\ 0 \le n \le N.$$

Note that the operators $\mathcal{A}_t^{\alpha}$ and δ_x^2 can be commuted to each other. Then using Lemma 3.1 yields

$$\mathcal{A}_x \delta_t^{\alpha,\lambda} U_i^n - \mathcal{A}_t^{\alpha} \delta_x^2 U_i^n = \mathcal{A}_t^{\alpha} \mathcal{A}_x F_i^n + R_i^n, \quad 1 \le i \le M-1,\ 1 \le n \le N, \tag{3.6}$$

where there exists a constant c_1 such that

$$|R_i^n| \le c_1(\tau^2 + h^4), \quad 1 \le i \le M-1,\ 1 \le n \le N. \tag{3.7}$$

Omitting the small terms R_i^n in (3.6), denoting u_i^n as the approximation of U_i^n and noticing the initial and boundary conditions

$$U_i^0 = 0, \quad 0 \le i \le M, \tag{3.8}$$

$$U_0^n = \phi(x_0, t_n), \qquad U_M^n = \phi(x_M, t_n), \quad 1 \le n \le N, \tag{3.9}$$

we obtain a (α, λ)-dependent compact difference scheme

$$\mathcal{A}_x \delta_t^{\alpha,\lambda} u_i^n - \mathcal{A}_t^{\alpha} \delta_x^2 u_i^n = \mathcal{A}_t^{\alpha} \mathcal{A}_x F_i^n, \quad 1 \le i \le M-1,\ 1 \le n \le N, \tag{3.10}$$

$$u_i^0 = 0, \quad 0 \le i \le M, \tag{3.11}$$

$$u_0^n = \phi(x_0, t_n), \qquad u_M^n = \phi(x_M, t_n), \quad 1 \le n \le N. \tag{3.12}$$

Remark 3.2. When $\lambda = \lambda(x)$, the problem (1.2)–(1.4) becomes the Feynman–Kac equation considered in [26]. In Section 5, we will show numerically that the adapted scheme, i.e., taking $\lambda_i = \lambda(x_i)$ in above scheme, is of second-order convergence in time and fourth-order convergence in space for the forward Feynman–Kac equation considered in [26].

4. Stability and convergence analysis

In this section, we shall give the stability and convergence analysis for the scheme (3.10)–(3.12).

Let $V_h = \{v \mid v = (v_0, \ldots, v_M)$ is a grid function on Ω_h and $v_0 = v_M = 0\}$. For any $u, v \in V_h$, we denote the maximum norm by $\|u\|_\infty = \max_{0 \le i \le M} |u_i|$ and define the discrete inner products and induced norm as

$$(u, v) = h \sum_{i=1}^{M-1} u_i v_i, \qquad \|u\| = \sqrt{(u, u)}.$$

Let

$$l_n^{\alpha} = \sum_{k=0}^{n} g_k^{\alpha}, \quad n \ge 0. \tag{4.1}$$

Then l_n^{α} are the coefficients of the power series expansion of the function $(1-z)^{\alpha-1}$, i.e.,

$$(1-z)^{\alpha-1} = \sum_{k=0}^{+\infty} l_k^{\alpha} z^k,$$

In fact, from $(1-z)^{\alpha} = (1-z) \cdot (1-z)^{\alpha-1}$, we have

$$\sum_{k=0}^{+\infty} g_k^{\alpha} z^k = (1-z) \sum_{k=0}^{+\infty} l_k^{\alpha} z^k = l_0^{\alpha} + \sum_{k=1}^{+\infty} (l_k^{\alpha} - l_{k-1}^{\alpha}) z^k.$$

Comparing the coefficients of power series expansion on both sides leads to the desired result. In addition, the coefficients l_n^{α} in (4.1) satisfy the following properties for $0 < \alpha < 1$,

$$\begin{cases} l_0^{\alpha} = 1, \quad l_1^{\alpha} = 1 - \alpha, \\ l_0^{\alpha} \ge l_1^{\alpha} \ge l_2^{\alpha} \ge l_3^{\alpha} \ge \cdots \ge 0. \end{cases} \tag{4.2}$$

And it has the lower bound, i.e.,

$$l_{n-1}^{\alpha} \ge \frac{1}{n^{\alpha} \Gamma(1-\alpha)}. \tag{4.3}$$

See Lemma 2.1 in [26] for details.

Prior to considering the stability and convergence of the scheme (3.10)–(3.12), we need to provide some auxiliary lemmas. Inspired by the work in [23], we first give the following lemma.

Lemma 4.1. *For a given sequence* $\{v^n\}_{n=0}^{\infty}$, *we have*

$$v^n\delta_t^{\alpha,\lambda}v^n \geq \frac{1}{2}e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2 + \frac{e^{-\frac{\alpha}{2}\lambda\tau}}{2l_0^\alpha}\tau^\alpha(\delta_t^{\alpha,\lambda}v^n)^2, \tag{4.4}$$

$$v^{n-1}\delta_t^{\alpha,\lambda}v^n \geq \frac{1}{2}e^{(1-\frac{\alpha}{2})\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2 - \frac{e^{(1-\frac{\alpha}{2})\lambda\tau}}{2(l_0^\alpha - l_1^\alpha)}\tau^\alpha(\delta_t^{\alpha,\lambda}v^n)^2, \tag{4.5}$$

where

$$\delta_t^{\alpha,2\lambda}(v^n)^2 = \frac{1}{\tau^\alpha}\sum_{k=0}^{n}g_k^{\alpha,2\lambda}(v^{n-k})^2.$$

Proof. Note that $g_k^{\alpha,\lambda} = e^{\lambda(\frac{\alpha}{2}-k)\tau}g_k^\alpha$. The expressions $\delta_t^{\alpha,\lambda}v^n$, $\delta_t^{\alpha,2\lambda}(v^n)^2$ can also be rewritten as

$$\delta_t^{\alpha,\lambda}v^n = e^{\lambda(\frac{\alpha}{2}-n)\tau}\frac{1}{\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha(e^{\lambda k\tau}v^k - e^{\lambda(k-1)\tau}v^{k-1}), \tag{4.6}$$

$$\delta_t^{\alpha,2\lambda}(v^n)^2 = e^{2\lambda(\frac{\alpha}{2}-n)\tau}\frac{1}{\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha[(e^{\lambda k\tau}v^k)^2 - (e^{\lambda(k-1)\tau}v^{k-1})^2], \tag{4.7}$$

where $v^{-1} = 0$. To simplify notation but without ambiguity, hereafter, we denote $v_\lambda^k := e^{\lambda k\tau}v^k$. Thus we have

$$\begin{aligned}
&e^{(2n-\frac{\alpha}{2})\lambda\tau}\left[v^n\delta_t^{\alpha,\lambda}v^n - \frac{1}{2}e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2\right] \\
&= v_\lambda^n\frac{1}{\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1}) - \frac{1}{\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1})\left(\frac{v_\lambda^k + v_\lambda^{k-1}}{2}\right) \\
&= \frac{1}{\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1})\left(v_\lambda^n - \frac{v_\lambda^k + v_\lambda^{k-1}}{2}\right) \\
&= \frac{1}{\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1})\left[\frac{v_\lambda^k - v_\lambda^{k-1}}{2} + \sum_{j=k+1}^{n}(v_\lambda^j - v_\lambda^{j-1})\right] \\
&= \frac{1}{2\tau^\alpha}\sum_{k=0}^{n}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1})^2 + \frac{1}{\tau^\alpha}\sum_{j=1}^{n}(v_\lambda^j - v_\lambda^{j-1})\sum_{k=0}^{j-1}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1}).
\end{aligned} \tag{4.8}$$

Denote

$$w_\lambda^j = \sum_{k=0}^{j-1}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1}), \quad 1 \leq j \leq n \tag{4.9}$$

and

$$w_\lambda^{n+1} = \sum_{k=0}^{n}l_{n-k}^\alpha(v_\lambda^k - v_\lambda^{k-1}) = \tau^\alpha e^{(n-\frac{\alpha}{2})\lambda\tau}\delta_t^{\alpha,\lambda}v^n. \tag{4.10}$$

Then it follows that

$$v_\lambda^0 - v_\lambda^{-1} = \frac{w_\lambda^1}{l_n^\alpha}; \qquad v_\lambda^j - v_\lambda^{j-1} = \frac{w_\lambda^{j+1} - w_\lambda^j}{l_{n-j}^\alpha}, \quad 1 \leq j \leq n. \tag{4.11}$$

Substituting (4.9)–(4.11) into (4.8) leads to

$$\begin{aligned}
&e^{(2n-\frac{\alpha}{2})\lambda\tau}\left[v^n\delta_t^{\alpha,\lambda}v^n - \frac{1}{2}e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2\right] \\
&= \frac{1}{2\tau^\alpha}l_n^\alpha\left(\frac{w_\lambda^1}{l_n^\alpha}\right)^2 + \frac{1}{2\tau^\alpha}\sum_{k=1}^{n}l_{n-k}^\alpha\left(\frac{w_\lambda^{k+1} - w_\lambda^k}{l_{n-k}^\alpha}\right)^2 + \frac{1}{\tau^\alpha}\sum_{j=1}^{n}\left(\frac{w_\lambda^{j+1} - w_\lambda^j}{l_{n-j}^\alpha}\right)w_\lambda^j \\
&= \frac{1}{2\tau^\alpha}\frac{(w_\lambda^{n+1})^2}{l_0^\alpha} + \frac{1}{2\tau^\alpha}\sum_{k=1}^{n}\left(\frac{1}{l_{n+1-k}^\alpha} - \frac{1}{l_{n-k}^\alpha}\right)(w_\lambda^k)^2.
\end{aligned} \tag{4.12}$$

Multiplying (4.12) by $e^{(\frac{\alpha}{2}-2n)\lambda\tau}$ and recalling (4.2), we have

$$v^n\delta_t^{\alpha,\lambda}v^n-\frac{1}{2}e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2\geq\frac{e^{(\frac{\alpha}{2}-2n)\lambda\tau}}{2\tau^\alpha}\frac{(w_\lambda^{n+1})^2}{l_0^\alpha}=\frac{e^{-\frac{\alpha}{2}\lambda\tau}}{2l_0^\alpha}\tau^\alpha(\delta_t^{\alpha,\lambda}v^n)^2.$$

Next, we prove the inequality (4.5). Considering the difference, using the notations (4.9)–(4.10) again and noting the equality (4.12), we have

$$\begin{aligned}
&e^{(2n-1-\frac{\alpha}{2})\lambda\tau}\left[v^{n-1}\delta_t^{\alpha,\lambda}v^n-\frac{1}{2}e^{(1-\frac{\alpha}{2})\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2+\frac{e^{(1-\frac{\alpha}{2})\lambda\tau}}{2(l_0^\alpha-l_1^\alpha)}\tau^\alpha(\delta_t^{\alpha,\lambda}v^n)^2\right]\\
&=e^{(2n-\frac{\alpha}{2})\lambda\tau}\left[v^n\delta_t^{\alpha,\lambda}v^n-\frac{1}{2}e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2\right]+\frac{\tau^\alpha}{2(l_0^\alpha-l_1^\alpha)}e^{(2n-\alpha)\lambda\tau}(\delta_t^{\alpha,\lambda}v^n)^2\\
&\quad-[e^{n\lambda\tau}v^n-e^{(n-1)\lambda\tau}v^{n-1}]e^{(n-\frac{\alpha}{2})\lambda\tau}\delta_t^{\alpha,\lambda}v^n\\
&=\frac{1}{2\tau^\alpha}\frac{(w_\lambda^{n+1})^2}{l_0^\alpha}+\frac{1}{2\tau^\alpha}\sum_{k=1}^{n}\left(\frac{1}{l_{n+1-k}^\alpha}-\frac{1}{l_{n-k}^\alpha}\right)(w_\lambda^k)^2+\frac{\tau^\alpha}{2(l_0^\alpha-l_1^\alpha)}\left(\frac{w_\lambda^{n+1}}{\tau^\alpha}\right)^2-\frac{(w_\lambda^{n+1}-w_\lambda^n)w_\lambda^{n+1}}{l_0^\alpha\tau^\alpha}\\
&=\frac{1}{\tau^\alpha}\left(\frac{1}{2(l_0^\alpha-l_1^\alpha)}-\frac{1}{2l_0^\alpha}\right)(w_\lambda^{n+1})^2+\frac{1}{\tau^\alpha}\frac{1}{l_0^\alpha}w_\lambda^nw_\lambda^{n+1}+\frac{1}{2\tau^\alpha}\left(\frac{1}{l_1^\alpha}-\frac{1}{l_0^\alpha}\right)(w_\lambda^n)^2+\frac{1}{2\tau^\alpha}\sum_{k=1}^{n-1}\left(\frac{1}{l_{n+1-k}^\alpha}-\frac{1}{l_{n-k}^\alpha}\right)(w_\lambda^k)^2\\
&=\frac{1}{2l_0^\alpha\tau^\alpha}\left(\sqrt{\frac{l_1^\alpha}{l_0^\alpha-l_1^\alpha}}w_\lambda^{n+1}+\sqrt{\frac{l_0^\alpha-l_1^\alpha}{l_1^\alpha}}w_\lambda^n\right)^2+\frac{1}{2\tau^\alpha}\sum_{k=1}^{n-1}\left(\frac{1}{l_{n+1-k}^\alpha}-\frac{1}{l_{n-k}^\alpha}\right)(w_\lambda^k)^2\\
&\geq 0,
\end{aligned}$$

which completes the proof. □

Lemma 4.2. *Given a sequence $\{v^n\}$ we have*

$$\mathcal{A}_t^\alpha v^n\cdot\delta_t^{\alpha,\lambda}v^n\geq\frac{1}{2}\left[\frac{\alpha}{2}e^{\lambda\tau}+\left(1-\frac{\alpha}{2}\right)\right]e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2+\frac{2-\alpha-e^{\lambda\tau}}{4}\tau^\alpha e^{-\frac{\alpha}{2}\lambda\tau}(\delta_t^{\alpha,\lambda}v^n)^2. \tag{4.13}$$

In particular, when $\alpha=1,\ \lambda=0$ it holds that

$$\mathcal{A}_tv^n\cdot\delta_tv^n:=\frac{v^n+v^{n-1}}{2}\cdot\frac{v^n-v^{n-1}}{\tau}=\frac{(v^n)^2-(v^{n-1})^2}{2\tau}.$$

Proof. From Lemma 4.1, we have

$$\begin{aligned}
\mathcal{A}_t^\alpha v^n\cdot\delta_t^{\alpha,\lambda}v^n&=\left(1-\frac{\alpha}{2}\right)v^n\delta_t^{\alpha,\lambda}v^n+\frac{\alpha}{2}v^{n-1}\delta_t^{\alpha,\lambda}v^n\\
&\geq\left(1-\frac{\alpha}{2}\right)e^{-\frac{\alpha}{2}\lambda\tau}\left[\frac{1}{2}\delta_t^{\alpha,2\lambda}(v^n)^2+\frac{\tau^\alpha}{2l_0^\alpha}(\delta_t^{\alpha,\lambda}v^n)^2\right]\\
&\quad+\frac{\alpha}{2}e^{(1-\frac{\alpha}{2})\lambda\tau}\left[\frac{1}{2}\delta_t^{\alpha,2\lambda}(v^n)^2-\frac{\tau^\alpha}{2(l_0^\alpha-l_1^\alpha)}(\delta_t^{\alpha,\lambda}v^n)^2\right]\\
&=\frac{1}{2}\left[\frac{\alpha}{2}e^{\lambda\tau}+\left(1-\frac{\alpha}{2}\right)\right]e^{-\frac{\alpha}{2}\lambda\tau}\delta_t^{\alpha,2\lambda}(v^n)^2+\left[\left(1-\frac{\alpha}{2}\right)\frac{1}{2l_0^\alpha}-\frac{\alpha}{2}\frac{e^{\lambda\tau}}{2(l_0^\alpha-l_1^\alpha)}\right]\tau^\alpha e^{-\frac{\alpha}{2}\lambda\tau}(\delta_t^{\alpha,\lambda}v^n)^2.
\end{aligned}$$

Substituting $l_0^\alpha=1$ and $l_1^\alpha=1-\alpha$ into above inequality leads to (4.13), which completes the proof. □

Lemma 4.3 ([35]). *For any $u, v\in V_h$, it holds that $(\mathcal{A}_xu, v)=(u, \mathcal{A}_xv)$.*

Lemma 4.4 ([35]). *For any $v\in V_h$, it holds that*

$$\frac{2}{3}\|v\|^2\leq(\mathcal{A}_xv, v)\leq\|v\|^2.$$

Since $\mathcal{A}_x$ is positive definite and self-adjoint, we can consider its square root denoted as Q_x, and have

$$(\mathcal{A}_xu, v)=(Q_xu, Q_xv). \tag{4.14}$$

Naturally, we define an equivalent norm as

$$\|v\|_A=\sqrt{(\mathcal{A}_xv, v)}=\sqrt{(Q_xv, Q_xv)}.$$

Lemma 4.5 *([35]). For any $v \in V_h$, it holds that $-(\delta_x^2 v, v) \geq C_\Omega \|v\|^2$, where C_Ω is a constant independent to the step size h but related to the domain Ω.*

Now we give a prior estimate for the difference scheme (3.10)–(3.12).

Theorem 4.6 (*Priori Estimate*). *Suppose $\{v_i^n\}$ be the solution of*

$$\mathcal{A}_x \delta_t^{\alpha,\lambda} v_i^n - \mathcal{A}_t^\alpha \delta_x^2 v_i^n = S_i^n, \quad 1 \leq i \leq M-1, \ 1 \leq n \leq N, \tag{4.15}$$

$$v_0^n = 0, \qquad v_M^n = 0, \quad 1 \leq n \leq N, \tag{4.16}$$

$$v_i^0 = v_0(x_i), \quad 0 \leq i \leq M. \tag{4.17}$$

If $2 - \alpha - e^{\lambda\tau} \geq 0$, then

$$\|v^n\|^2 \leq \frac{3}{2} e^{2|\lambda|T} \|v^0\|^2 + \frac{3\Gamma(1-\alpha)T^\alpha e^{2|\lambda|T}}{C_\Omega} \max_{0 \leq n \leq N} \|S^n\|^2 \tag{4.18}$$

for $1 < n \leq N$, where $v_0(x_0) = v_0(x_M) = 0$, $\|S^n\| = \sqrt{h \sum_{i=1}^{M-1} (S_i^n)^2}$.

Proof. Taking the inner product of (4.15) with $\mathcal{A}_t^\alpha v^n$, we have

$$(\mathcal{A}_x \delta_t^{\alpha,\lambda} v^n, \mathcal{A}_t^\alpha v^n) - (\mathcal{A}_t^\alpha \delta_x^2 v^n, \mathcal{A}_t^\alpha v^n) = (S^n, \mathcal{A}_t^\alpha v^n). \tag{4.19}$$

By (4.14), for the first term on the left-hand side of (4.19), we get

$$(\mathcal{A}_x \delta_t^{\alpha,\lambda} v^n, \mathcal{A}_t^\alpha v^n) = (Q_x \delta_t^{\alpha,\lambda} v^n, Q_x \mathcal{A}_t^\alpha v^n) = (\delta_t^{\alpha,\lambda} Q_x v^n, \mathcal{A}_t^\alpha Q_x v^n).$$

By Lemma 4.2 and assumption $2 - \alpha - e^{\lambda\tau} \geq 0$, we have

$$\begin{aligned}(\delta_t^{\alpha,\lambda} Q_x v^n, \mathcal{A}_t^\alpha Q_x v^n) &= h \sum_{i=1}^{M-1} \delta_t^{\alpha,\lambda} (Q_x v^n)_i \cdot \mathcal{A}_t^\alpha (Q_x v^n)_i \\ &\geq \frac{1}{2} e^{-\frac{\alpha}{2}\lambda\tau} \left[\frac{\alpha}{2} e^{\lambda\tau} + \left(1 - \frac{\alpha}{2}\right)\right] h \sum_{i=1}^{M-1} \delta_t^{\alpha,2\lambda} (Q_x v^n)_i^2.\end{aligned} \tag{4.20}$$

For the second term on the left-hand side, from Lemma 4.5, we obtain

$$-(\mathcal{A}_t^\alpha \delta_x^2 v^n, \mathcal{A}_t^\alpha v^n) = -(\delta_x^2 \mathcal{A}_t^\alpha v^n, \mathcal{A}_t^\alpha v^n) \geq C_\Omega \|\mathcal{A}_t^\alpha v^n\|^2. \tag{4.21}$$

As to the term on the right-hand side, in view of Lemma 4.3 we have

$$(S^n, \mathcal{A}_t^\alpha v^n) \leq \|S^n\| \cdot \|\mathcal{A}_t^\alpha v^n\| \leq \frac{1}{4C_\Omega} \|S^n\|^2 + C_\Omega \|\mathcal{A}_t^\alpha v^n\|^2. \tag{4.22}$$

Substituting (4.20)–(4.22) into (4.19), we obtain

$$\frac{1}{2} e^{-\frac{\alpha}{2}\lambda\tau} \left[\frac{\alpha}{2} e^{\lambda\tau} + \left(1 - \frac{\alpha}{2}\right)\right] h \sum_{i=1}^{M-1} \delta_t^{\alpha,2\lambda} (Q_x v^n)_i^2 \leq \frac{1}{4C_\Omega} \|S^n\|^2.$$

Since $\frac{\alpha}{2} e^{\lambda\tau} + (1 - \frac{\alpha}{2}) \geq \frac{1}{2}$, we have

$$e^{-\frac{\alpha}{2}\lambda\tau} h \sum_{i=1}^{M-1} \delta_t^{\alpha,2\lambda} (Q_x v^n)_i^2 \leq \frac{1}{C_\Omega} \|S^n\|^2.$$

Consequently, by (4.7), it follows that

$$\begin{aligned} l_0^\alpha \|v_\lambda^n\|_A^2 &\leq \sum_{k=1}^{n-1} (l_{n-k-1}^\alpha - l_{n-k}^\alpha) \|v_\lambda^k\|_A^2 + (l_{n-1}^\alpha - l_n^\alpha) \|v_\lambda^0\|_A^2 + \frac{\tau^\alpha}{C_\Omega} e^{(2n-\frac{\alpha}{2})\lambda\tau} \|S^n\|^2 \\ &\leq \sum_{k=1}^{n-1} (l_{n-k-1}^\alpha - l_{n-k}^\alpha) \|v_\lambda^k\|_A^2 + l_{n-1}^\alpha \left(\|v_\lambda^0\|_A^2 + \frac{\tau^\alpha}{C_\Omega l_{n-1}^\alpha} e^{(2n-\frac{\alpha}{2})\lambda\tau} \|S^n\|^2 \right) \\ &\leq \sum_{k=1}^{n-1} (l_{n-k-1}^\alpha - l_{n-k}^\alpha) \|v_\lambda^k\|_A^2 + l_{n-1}^\alpha \left(\|v_\lambda^0\|^2 + \frac{\Gamma(1-\alpha)T^\alpha}{C_\Omega} e^{(2n-\frac{\alpha}{2})\lambda\tau} \|S^n\|^2 \right), \quad 1 \leq n \leq N, \end{aligned} \tag{4.23}$$

where we have used the estimate (4.3) in the last inequality. Denote

$$E^N = \|v_\lambda^0\|^2 + \frac{\Gamma(1-\alpha)T^\alpha}{C_\Omega} \max_{1\le n\le N} e^{(2n-\frac{\alpha}{2})\lambda\tau} \max_{1\le n\le N} \|S^n\|^2.$$

The inequality (4.23) is simplified to

$$l_0^\alpha \|v_\lambda^n\|_A^2 \le \sum_{k=1}^{n-1} (l_{n-k-1}^\alpha - l_{n-k}^\alpha)\|v_\lambda^k\|_A^2 + l_{n-1}^\alpha E^N, \quad 1 \le n \le N. \tag{4.24}$$

Next we prove the following inequality

$$\|v_\lambda^n\|_A^2 \le E^N, \quad 1 \le n \le N \tag{4.25}$$

by the mathematical induction method. Obviously, it follows from (4.24) that the equality (4.25) holds for $n = 1$. Suppose that (4.25) still holds for $n = 1, 2, \dots, m$. From (4.24) at $n = m + 1$, we have

$$\begin{aligned} l_0^\alpha \|v_\lambda^{m+1}\|_A^2 &\le \sum_{k=1}^{m} (l_{m-k}^\alpha - l_{m+1-k}^\alpha)\|v_\lambda^k\|_A^2 + l_m^\alpha E^N \\ &\le \sum_{k=1}^{m} (l_{m-k}^\alpha - l_{m+1-k}^\alpha)E^N + l_m^\alpha E^N = l_0^\alpha E^N, \end{aligned}$$

which leads to (4.25).

It follows from Lemma 4.4 that

$$\frac{2}{3} e^{2\lambda n\tau}\|v^n\|^2 = \frac{2}{3}\|v_\lambda^n\|^2 \le \|v_\lambda^n\|_A^2 \le E^N.$$

Thus

$$\begin{aligned} \|v^n\|^2 &\le \frac{3}{2} e^{-2\lambda n\tau} E^N \\ &\le \frac{3}{2} e^{-2\lambda n\tau}\left(\|v^0\|^2 + \frac{\Gamma(1-\alpha)T^\alpha}{C_\Omega} \max_{1\le n\le N} e^{(2n-\frac{\alpha}{2})\lambda\tau} \max_{1\le n\le N}\|S^n\|^2\right) \\ &\le \frac{3}{2} e^{2|\lambda|T}\|v^0\|^2 + \frac{3\Gamma(1-\alpha)T^\alpha}{C_\Omega} e^{2|\lambda|T} \max_{1\le n\le N}\|S^n\|^2, \quad 1 \le n \le N. \end{aligned}$$

This completes the proof. □

Using Theorem 4.6, it is ready to obtain the following result.

Theorem 4.7 (*Stability*)**.** *The difference scheme (3.10)–(3.12) is unconditionally stable with respect to the initial value and right-hand term.*

We now turn to the convergence of the difference scheme (3.10)–(3.12).

Theorem 4.8 (*Convergence*)**.** *Assume that $u(x,t) \in C^{6,3}(\Omega \times [0,T])$ be the solution of the problem (1.2)–(1.4), and $\{u_i^n\}$ be the solution of difference scheme (3.10)–(3.12). We further assume that zero extended function $u(x,t)$ satisfies the assumptions in Theorem 2.3. Let $e_i^n = u(x_i,t_n) - u_i^n$, $0 \le i \le M$, $0 \le n \le N$. Then the following estimate*

$$\|e^n\| \le \sqrt{\frac{3\Gamma(1-\alpha)e^{2|\lambda|T}T^\alpha(b-a)}{C_\Omega}}\, c_1(\tau^2 + h^4), \quad 1 \le n \le N$$

holds, where C_Ω is defined as that in Lemma 4.5.

Proof. Subtracting (3.10)–(3.12) from (3.6), (3.8)–(3.9) respectively, we get the error equations

$$\begin{aligned} &\mathcal{A}_x \delta_t^{\alpha,\lambda} e_i^n - \mathcal{A}_t^\alpha \delta_x^2 e_i^n = R_i^n, \quad 1 \le i \le M-1,\ 1 \le n \le N, \\ &e_0^n = 0, \qquad e_M^n = 0, \quad 1 \le n \le N, \\ &e_i^0 = 0, \quad 0 \le i \le M. \end{aligned}$$

It follows from Theorem 4.6 and the truncation error estimate (3.7) that

$$\begin{aligned}\|e^n\|^2 &\le \frac{3\Gamma(1-\alpha)e^{2|\lambda|T}T^\alpha}{C_\Omega}\max_{0\le n\le N}\|R^n\|^2\\ &\le \frac{3\Gamma(1-\alpha)e^{2|\lambda|T}T^\alpha(b-a)}{C_\Omega}c_1^2(\tau^2+h^4)^2,\quad 1\le n\le N.\end{aligned}$$

This completes the proof. □

5. An improved algorithm

This section presents an improved algorithm for the problem (1.2)–(1.4) with nonsmooth solution. To begin with this section, we first introduce the following lemma.

Lemma 5.1. *Let $f(t)=e^{-\lambda t}t^\beta,\ \beta>0$. Then*

$$\left(1-\frac{\alpha}{2}\right)[{}_{-\infty}D_t^{\alpha,\lambda}f(t)]_{t=t_n}+\frac{\alpha}{2}[{}_{-\infty}D_t^{\alpha,\lambda}f(t)]_{t=t_{n-1}}=\frac{1}{\tau^\alpha}\sum_{k=0}^{n}g_k^{\alpha,\lambda}f(t_{n-k})+\mathcal{O}(t_n^{\beta-\alpha-2}\tau^2)$$

uniformly holds in $t\in\mathbb{R}$ as $\tau\to 0$, where $g_k^{\alpha,\lambda}=e^{-(k-\frac{\alpha}{2})\lambda\tau}g_k^\alpha$.

The proof of above lemma is similar to [25] and here we skip it.

To fix the idea, let us first consider the fractional ordinary differential equation with substantial derivative as below

$${}_0D_t^{\alpha,\lambda}u(t)=\mu u(t)+F(t). \tag{5.1}$$

We can seek its solution of the following form

$$u(t)=\sum_{j,k=0}^{+\infty}c_{j,k}e^{-\lambda t}t^{k+j\alpha}, \tag{5.2}$$

which can be derived by the method of power series. Indeed, suppose that the right-hand side function F is sufficiently smooth and has the power series expansion of the form below

$$F(t)=\sum_{k=0}^{+\infty}F_ke^{-\lambda t}t^k. \tag{5.3}$$

Inserting (5.2) and (5.3) into (5.1) leads to

$$\sum_{j,k=0}^{+\infty}c_{j,k}{}_0D_t^{\alpha,\lambda}(e^{-\lambda t}t^{k+j\alpha})=\mu\sum_{j,k=0}^{+\infty}c_{j,k}e^{-\lambda t}t^{k+j\alpha}+\sum_{k=0}^{+\infty}F_ke^{-\lambda t}t^k.$$

Consequently

$$\sum_{j,k=0}^{+\infty}c_{j,k}e^{-\lambda t}\frac{\Gamma(k+1+j\alpha)}{\Gamma(k+1+(j-1)\alpha)}t^{k+(j-1)\alpha}=\mu\sum_{j,k=0}^{+\infty}c_{j,k}e^{-\lambda t}t^{k+j\alpha}+\sum_{k=0}^{+\infty}F_ke^{-\lambda t}t^k, \tag{5.4}$$

where we have used the formula

$${}_0D_t^{\alpha,\lambda}(e^{-\lambda t}t^{k+j\alpha})=e^{-\lambda t}\frac{\Gamma(k+1+j\alpha)}{\Gamma(k+1+(j-1)\alpha)}t^{k+(j-1)\alpha}.$$

Comparing the coefficients of both sides of identity (5.4) can solve $c_{j,k}$, the coefficients to be determined.

Now we turn our attention back to the TFSDE (1.2)–(1.4). From the aforementioned discussion, it makes sense to suppose the solution has the following structure:

$$u(\mathbf{x},t)=\sum_{j,k=0}^{+\infty}c_{j,k}(\mathbf{x})e^{-\lambda(\mathbf{x})t}t^{k+j\alpha}. \tag{5.5}$$

From the asymptotic behavior of the solution near the original point $t=0$ in (5.5), we can clearly see, by Lemma 5.1, that the expected convergence order of the scheme proposed in the previous section may decrease correspondingly and thus the accuracy will deteriorate meantime. To make up for the lost accuracy, we have to turn to other approaches. One of the natural ideas occurs to us: if we can remove or separate the singular part from the candidate solution, then the remaining part has desired regularity to satisfy the necessary smoothness assumptions. However, this seems to be ideal but cannot work in practice since the coefficients $c_{j,k}$ is unknown and difficult to calculate. An efficient approach firstly proposed by Lubich [25] is to add starting quadrature to make sure that the corrected scheme is accurate for the power function t^{β}, $\beta \in \Theta$, where $\Theta = \{\beta \mid \beta = k + j\alpha : j, k \in \mathbb{N}, \beta \le 2+\alpha\}$. Following the spirit of Lubich [25], by Lemma 5.1 we get the following semi-discrete correction scheme

$$\delta_t^{\alpha,\lambda} u(\mathbf{x}, t_n) + \sum_{k=0}^{S} w_{n,k}^{\alpha,\lambda} u(\mathbf{x}, t_k) = \mathcal{A}_t^{\alpha} \Delta u(\mathbf{x}, t_n) + \mathcal{A}_t^{\alpha} F(\mathbf{x}, t_n) + \mathcal{O}(\tau^2), \quad 1 \le n \le N, \tag{5.6}$$

for the problem (1.2)–(1.4) with solution in the form of (5.5), where S is the number of elements of the set Θ and the starting weights $w_{n,k}^{\alpha,\lambda}$ can be computed from the Vandermonde type system

$$\sum_{k=0}^{S} w_{n,k}^{\alpha,\lambda} t_k^{\beta_j} e^{-\lambda t_k} = \left(1 - \frac{\alpha}{2}\right) \frac{\Gamma(\beta_j+1)}{\Gamma(\beta_j+1-\alpha)} t_n^{\beta_j-\alpha} e^{-\lambda t_n} + \frac{\alpha}{2} \frac{\Gamma(\beta_j+1)}{\Gamma(\beta_j+1-\alpha)} t_{n-1}^{\beta_j-\alpha} e^{-\lambda t_{n-1}} - \frac{1}{\tau^{\alpha}} \sum_{k=0}^{n} g_k^{\alpha,\lambda} t_n^{\beta_j} e^{-\lambda t_k}, \quad j = 0, \dots, S. \tag{5.7}$$

Instead of studying the theory of the improved algorithm, we will provide a two-dimensional example to show its validity in next section, where a fully discretized compact finite scheme for the two-dimensional TFSDE is also given; see Example 6.3.

Remark 5.2. Based on the pitfalls in fast numerical solvers for fractional differential equations studied in [36], it is known that the linear system (5.7) is ill-posed, which may result in the reduced efficiency of the algorithm (5.6). However, using a few correction terms can significantly increase the accuracy for problems with low regularity. It will not be computationally expensive to calculate the necessary starting weights; see also [37].

6. Numerical examples

In this section, we give some numerical results to illustrate the performance of the proposed scheme and verify the theoretical prediction. In Example 6.1, a prototypical equation is considered to show the convergence order of the proposed second-order approximation (2.9) with or without the smoothness assumptions in Theorem 2.3. Example 6.2 provides a comparison between the proposed scheme (3.10)–(3.12) and the scheme in [26], for solving the backward Feynman–Fac equation (6.1). In Example 6.3, we illustrate efficiency of the improved algorithm by solving a two-dimensional TFSDE with nonsmooth solution.

Example 6.1. Consider the following prototypical equation

$${}_0D_t^{\alpha,\lambda} u(t) = f(t),$$

with $u(0)$ and the source term $f(t)$ such that the equation admits the solution $u(t) = e^{-\lambda t}(t^3 + t^{\nu})$, and $0 < \alpha < 1$. We take $\lambda = 0.5$ and change ν to test the convergence order of the approximation (2.9) for the problem with different regularity.

Denote

$$E(\tau) = \max_{1 \le n \le N} |u^n - U^n|.$$

In this example $Rate = \log_2 \frac{E(2\tau)}{E(\tau)}$.

Table 6.1 displays that the approximation (2.9) can obtain second-order accuracy in uniform maximum norm when $\nu = 2.5$ and 2, while the convergence order decays with the decrease of ν evidently. The reduction of accuracy implies that some additional assumptions are needed to get second-order convergence for the approximation (2.9), e.g., the vanishing derivatives $u_t(0) = 0$. To keep the second-order convergence of the approximation (2.9), we make an assumption of the extended solution $\tilde{u}(t) \in \mathscr{C}^{2+\alpha}(\mathbb{R})$ in this paper. To some extent the assumption may be too strict, so we have considered the use of correction terms in the proposed schemes for problems with low regularity; see Section 5 for the improved schemes and Example 6.3 for the corresponding numerical results.

Example 6.2. Consider the backward fractional Feynman–Kac equation presented in [26]

$${}_0\partial_t^{\alpha,\lambda(x)} [P(x,\rho,t) - e^{-\rho U(x) t} P(x,\rho,0)] = \kappa_{\alpha} \partial_x^2 P(x,\rho,t) + f(x,t) \tag{6.1}$$

on a finite domain $0 < x < 1$, $0 < t \le 1$, with the coefficients $\kappa_{\alpha} = 0.5$, and $\lambda(x) = \rho U(x)$, $U(x) = x$, $\rho = 1 + \sqrt{-1}$; the forcing function

$$f(x,t) = -\kappa_{\alpha} e^{-\rho x t}(t^{3+\alpha} + 1)(\rho^2 t^2 \sin(\pi x) - 2\pi \rho t \cos(\pi x) - \pi^2 \sin(\pi x)), + \frac{\Gamma(4+\alpha)}{\Gamma(4)} e^{-\rho x t} t^3 \sin(\pi x). \tag{6.2}$$

the initial condition $P(x,\rho,0) = \sin(\pi x)$, and the boundary conditions $P(0,\rho,t) = P(1,\rho,t) = 0$. The exact solution is given by $P(x,\rho,t) = e^{-\rho x t}(t^{3+\alpha} + 1)\sin(\pi x)$.

Table 6.1
Error and convergence order of the approximation (2.9) for $u(t)$ with different regularity (Example 6.1).

	τ	$\alpha = 0.2$		$\alpha = 0.5$		$\alpha = 0.8$	
		$E(\tau)$	Rate	$E(\tau)$	Rate	$E(\tau)$	Rate
$\nu = 2.5$	1/16	1.9225e−4		4.7884e−4		7.5901e−4	
	1/32	4.8101e−5	2.00	1.2002e−4	1.99	1.9083e−4	2.00
	1/64	1.2029e−5	2.00	3.0043e−5	2.00	4.7871e−5	2.00
	1/128	3.0076e−6	2.00	7.5152e−6	2.00	1.1993e−5	2.00
$\nu = 2$	1/16	1.5725e−4		3.8400e−4		5.6264e−4	
	1/32	3.9392e−5	2.00	9.6827e−5	1.99	1.4297e−4	1.98
	1/64	9.8586e−6	2.00	2.4348e−5	1.99	3.6235e−5	1.98
	1/128	2.4661e−6	2.00	6.1116e−6	1.99	9.1649e−6	1.98
$\nu = 1.5$	1/16	1.3578e−4		3.1355e−4		3.0475e−4	
	1/32	3.6556e−5	1.89	7.8536e−5	2.00	1.2018e−4	1.34
	1/64	1.2691e−5	1.53	1.9651e−5	2.00	4.4176e−5	1.44
	1/128	4.4625e−6	1.51	4.9148e−6	2.00	1.5849e−5	1.48
$\nu = 1$	1/16	8.0608e−4		3.1355e−4		1.0800e−3	
	1/32	4.0503e−4	0.99	7.0492e−4	1.00	5.2210e−4	1.05
	1/64	2.0355e−4	0.99	3.5386e−4	0.99	2.6071e−4	1.00
	1/128	1.0211e−4	1.00	1.7745e−4	1.00	1.3082e−4	0.99
$\nu = 0.5$	1/16	1.0492e−2		2.7597e−2		4.9525e−2	
	1/32	7.5289e−3	0.48	1.9804e−2	0.48	3.5543e−2	0.48
	1/64	5.3646e−3	0.49	1.4111e−2	0.49	2.5327e−2	0.49
	1/128	3.8081e−3	0.49	1.0017e−2	0.49	1.7978e−2	0.49

Notice that the initial value is not equal to zero. So we have made the transformation

$$u(x,t) = P(x,\rho,t) - e^{-\rho x t}P(x,\rho,0).$$

Actually, replacing the average operators $\mathcal{A}_t^\alpha$ and $\mathcal{A}_x$ in (3.10)–(3.11) by identity operators in temporal and spatial directions respectively, we can obtain the following scheme in [26] as below

$$\delta_t^{\alpha,\lambda_i}u_i^n - \delta_x^2 u_i^n = F_i^n, \quad 1 \le i \le M-1,\ 1 \le n \le N, \tag{6.3}$$

$$u_i^0 = u_0(x_i), \quad 0 \le i \le M, \tag{6.4}$$

$$u_0^n = \phi_a(x_0,t_n), \qquad u_M^n = \phi_b(x_M,t_n), \quad 1 \le n \le N. \tag{6.5}$$

Define the error

$$E_1(\tau,h) = \max_{1\le i\le M-1}|u(x_i,t_N) - u_i^N|,$$

where $u(x_i,t_N)$ represents the exact solution and u_i^N is the numerical solution with the mesh step-sizes h and τ at the grid point (x_i,t_N). Assume

$$E_1(\tau,h) = O(\tau^p) + O(h^q).$$

If τ is sufficiently small, then $E_1(\tau,h) \approx O(h^q)$. Consequently, $\frac{E_1(\tau,2h)}{E_1(\tau,h)} \approx 2^q$ and $q \approx \log_2\left(\frac{E_1(\tau,2h)}{E_1(\tau,h)}\right)$ is the convergence order with respect to the spatial step size. Likewise, the convergence order in time can be taken as $p \approx \log_2(\frac{E_1(2\tau,h)}{E_1(\tau,h)})$ with sufficiently small h. Tables 6.2 and 6.3 list the errors and convergence orders of our scheme, showing that it is of second-order convergence in time and fourth-order convergence in space respectively. This is in a good agreement with our theoretical results. Evidently, we can see from Fig. 6.1 that our proposed scheme displays much higher accuracy and enjoys advantage over the scheme (6.3)–(6.5) presented in [26]. Table 6.4 further shows that when the two schemes generate the same accuracy, our proposed scheme needs fewer temporal and spatial grid points and less CPU time than that of scheme (6.3)–(6.5).

Example 6.3. Consider the following two dimensional backward fractional Feynman–Kac equations

$${}_0\partial_t^{\alpha,\lambda(x,y)}[u(x,y,t) - e^{-\lambda(x,y)t}u(x,y,0)] = \Delta u(x,y,t) + F(x,y,t) \tag{6.6}$$

on a finite domain $\Omega = (0,1)\times(0,1), 0 < t \le 1$, and $\lambda(x,y) = 0.01(x+y)$. We take the initial condition $u(x,y,0) = \sin(\pi x)\sin(\pi y)$, and the boundary condition $u(x,y,t) = 0$ for $(x,y) \in \partial\Omega$. The exact solution is

$$u(x,y,t) = e^{-\lambda(x,y)t}(1 + t^\alpha + t^{2\alpha} + t^3)\sin(\pi x)\sin(\pi y).$$

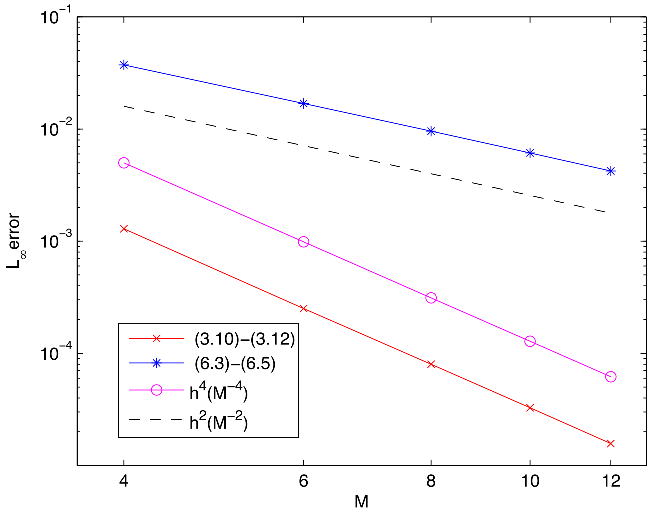

Fig. 6.1. Convergence order and error comparison between the scheme (3.10)–(3.12) and the scheme (6.3)–(6.5) in [26] with $\alpha = 0.5$ for solving Eq. (6.1) at $t = 1$. In all cases, we set $N = M^2$ (Example 6.2).

Table 6.2
Error and convergence order of the scheme (3.10)–(3.12) in time with a fixed space step-size $h = 1/40$ and $\lambda(x) = (1+\sqrt{-1})x$ (Example 6.2).

τ	$\alpha = 0.2$		$\alpha = 0.5$		$\alpha = 0.8$	
	$E_1(\tau, h)$	*Rate*	$E_1(\tau, h)$	*Rate*	$E_1(\tau, h)$	*Rate*
1/5	5.1150e−3		1.3602e−2		2.1793e−2	
1/10	1.3025e−3	1.97	3.4574e−3	1.98	5.5020e−3	1.99
1/20	3.2845e−4	1.99	8.7149e−4	1.99	1.3819e−3	1.99
1/40	8.2375e−5	2.00	2.1870e−4	1.99	3.4619e−4	2.00

Table 6.3
Error and convergence order of the scheme (3.10)–(3.12) in space with a fixed time step $\tau = 1/10\,000$ and $\lambda(x) = (1+\sqrt{-1})x$ (Example 6.2).

h	$\alpha = 0.2$		$\alpha = 0.5$		$\alpha = 0.8$	
	$E_1(\tau, h)$	*Rate*	$E_1(\tau, h)$	*Rate*	$E_1(\tau, h)$	*Rate*
1/4	2.0681e−03		1.7956e−03		1.4439e−03	
1/8	1.2566e−04	4.04	1.1059e−04	4.02	9.0999e−05	3.99
1/16	7.9126e−06	3.99	6.9117e−06	4.00	5.6411e−06	4.01
1/32	4.9271e−07	4.01	4.2904e−07	4.01	3.4901e−07	4.01
1/64	2.9927e−08	4.04	2.4756e−08	4.12	1.8798e−08	4.21

Table 6.4
A comparison between the scheme (3.10)–(3.12) and the scheme (6.3)–(6.5) in [26] for different α and step sizes for solving Eq. (6.1) (Example 6.2).

	The scheme (3.10)–(3.12)				The scheme (6.3)–(6.5)			
	N	M	$E_1(\tau, h)$	CPU (s)	N	M	$E_1(\tau, h)$	CPU (s)
$\alpha = 0.1$	16	4	1.9804e−3	0.0151	256	16	2.2831e−3	1.0427
	36	6	3.8109e−4	0.0340	1296	36	4.5106e−4	50.9968
	64	8	1.1946e−4	0.0661	4096	64	1.4269e−4	1484.3471
$\alpha = 0.5$	16	4	1.2906e−3	0.0090	256	16	2.3822e−3	0.9892
	36	6	2.5103e−4	0.0262	1296	36	4.6994e−4	50.6735
	64	8	7.9988e−5	0.0671	4096	64	1.4863e−4	1491.8938
$\alpha = 0.9$	16	4	1.6037e−3	0.0077	256	16	2.8498e−3	0.9932
	36	6	3.4057e−4	0.0261	1296	36	5.6214e−4	51.8453
	64	8	1.0771e−4	0.0687	4096	64	1.7779e−4	1471.3060

For spatial approximation, take two integers M_1, M_2 and let $h_1 = 1/M_1, h_2 = 1/M_2, x_i = ih_1, 0 \le i \le M_1, y_j = jh_2, 0 \le j \le M_2$. Let $\bar{\Omega}_h = \{(x_i, y_j) | 0 \le i \le M_1,\ 0 \le j \le M_2\}$, and $\Omega_h = \bar{\Omega}_h \cap \Omega$, and $\partial\Omega_h = \bar{\Omega}_h \cap \partial\Omega$. For any grid function

Table 6.5
Error and convergence order of the scheme (6.7)–(6.9) for the 2D problem (6.6). $\alpha = 0.2$, $h_1 = h_2 = 1/60$; S denotes the number of correction terms (Example 6.3).

N	$S=0$		$S=1$		$S=2$		$S=3$	
	$E_2(\tau,h_1,h_2)$	Rate	$E_2(\tau,h_1,h_2)$	Rate	$E_2(\tau,h_1,h_2)$	Rate	$E_2(\tau,h_1,h_2)$	Rate
4	9.32e−3		8.86e−4		6.68e−4		1.47e−3	
8	8.68e−3	0.10	2.76e−4	1.68	1.95e−4	1.78	2.34e−4	2.65
16	8.03e−3	0.11	2.02e−4	0.45	5.09e−5	1.94	5.31e−5	2.14
32	7.43e−3	0.11	1.70e−4	0.25	1.32e−5	1.95	1.33e−5	2.00

$v = \{v_{i,j} | 0 \le i \le M_1, 0 \le j \le M_2\}$, denote

$$\delta_x v_{i-\frac{1}{2},j} = \frac{1}{h_1}(v_{i,j} - v_{i-1,j}), \qquad \delta_x^2 v_{i,j} = \frac{1}{h_1}(\delta_x v_{i+\frac{1}{2},j} - \delta_x v_{i-\frac{1}{2},j}).$$

Similar notations $\delta_y v_{i,j-\frac{1}{2}}$, $\delta_y^2 v_{i,j}$ can be defined. The spatial average operators are defined as

$$\mathcal{A}_x v_{i,j} = \begin{cases} \frac{1}{12}(v_{i-1,j} + 10v_{i,j} + v_{i+1,j}), & 1 \le i \le M_1 - 1,\ \ 0 \le j \le M_2, \\ v_{i,j}, \quad i = 0 \text{ or } M_1,\ \ 0 \le j \le M_2, \end{cases}$$

$$\mathcal{A}_y v_{i,j} = \begin{cases} \frac{1}{12}(v_{i,j-1} + 10v_{i,j} + v_{i,j+1}), & 1 \le j \le M_2 - 1,\ 0 \le i \le M_1, \\ v_{i,j}, \quad j = 0 \text{ or } M_2,\ \ 0 \le i \le M_1. \end{cases}$$

By generalizing the improved scheme (5.6), we present a compact difference scheme with correction terms in time for the two-dimensional equation (6.6)

$$\mathcal{A}_x\mathcal{A}_y[\delta_t^{\alpha,\lambda} u_{i,j}^n + \sum_{k=0}^{S} w_{n,k}^{\alpha,\lambda} u_{i,j}^n] - \mathcal{A}_t^{\alpha}\mathcal{A}_y\delta_x^2 u_{i,j}^n - \mathcal{A}_t^{\alpha}\mathcal{A}_x\delta_y^2 u_{i,j}^n = \mathcal{A}_t^{\alpha}\mathcal{A}_x\mathcal{A}_y F_{i,j}^n, \quad (x_i, y_j) \in \Omega_h, \ \ 1 \le n \le N, \tag{6.7}$$

$$u_{i,j}^0 = u_0(x_i, y_j), \quad (x_i, y_j) \in \bar{\Omega}_h, \tag{6.8}$$

$$u_{i,j}^n = \phi(x_i, y_j, t_n), \quad (x_i, y_j) \in \partial\Omega_h,\ \ 1 \le n \le N. \tag{6.9}$$

Denote

$$E_2(\tau, h_1, h_2) = \max_{1 \le n \le N} \|u(\cdot, \cdot, t_n) - u^n\|_\infty.$$

Table 6.5 shows that the errors behave well and convergence order is augmented up to two with the increase of the number of correction terms, which indicates the efficiency and validity of our improved algorithm.

7. Conclusion

We have proposed a second-order approximation for the fractional substantial derivative and applied it to solve the time-fractional substantial diffusion equation. By combining the fourth-order compact finite difference approximation, a fully discrete Grünwald–Letnikov-formula-based compact difference scheme has been presented. It has been proved that the proposed scheme is unconditionally stable and of second-order convergence in time and fourth-order convergence in space.

We have numerically showed that our proposed scheme can reach the predicted accuracy when solving a problem with smooth solution. Compared with the scheme proposed in [26] for solving the backward Feynman–kac fractional equation, our scheme requires less storage and computational cost for the same accuracy. While if the solution is not smooth enough, we have illustrated in Example 6.1 that our proposed scheme loses its accuracy to some extent. To overcome this difficulty, we followed the idea of Lubich [25] and introduced the corresponding starting quadratures of substantial version. We have proposed an improved algorithm by applying the correction terms to increase the accuracy of the scheme near the origin and recover the second-order accuracy in time for problems with nonsmooth solution, which has been demonstrated by Example 6.3.

By the modified Grünwald derivative and the shifted Grünwald–Letnikov-formula, we have presented a weighted and shifted substantial Grünwald formula and given its asymptotic expansion, which is essential to derive the second-order approximation for the fractional substantial derivative. The proposed weighted average method is an efficient tool to get high-order scheme, not limited to the problem under consideration in this study. It can also be extended and applied to solve tempered fractional equations, which have attracted considerable interest recently; see [27,38]. It should be also pointed out that our scheme is consistent with the Crank–Nicolson scheme when the fractional derivatives reduce to the standard operators, which is one of attractive features of our proposed scheme.

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References

[1] I. Bronstein, Y. Israel, E. Kepten, S. Mai, Y. Shav-Tal, E. Barkai, Y. Garini, Transient anomalous diffusion of telomeres in the nucleus of mammalian cells, Phys. Rev. Lett. 103 (2009) 018102.
[2] G.G. Cabal, A. Genovesio, S.R. Navarro, C. Zimmer, O. Gadal, A. Lesne, H. Buc, F.F. Fournier, J.-C.O. Marin, E.C. Hurt, U. Nehrbass, SAGA interacting factors confine sub-diffusion of transcribed genes to the nuclear envelope, Nature 441 (2006) 770–773.
[3] A. Comtet, J. Desbois, C. Texier, Functionals of Brownian motion, localization and metric graphs, J. Phys. A: Math. Gen. 38 (2005) R341–R383.
[4] D. Kleinhans, R. Friedrich, Continuous-time random walks: Simulation of continuous trajectories, Phys. Rev. E 76 (2007) 061102.
[5] S. Carmi, E. Barkai, Fractional Feynman–Kac equation for weak ergodicity breaking, Phys. Rev. E 84 (2011)) 061104.
[6] S. Carmi, L. Turgeman, E. Barkai, On distributions of functionals of anomalous diffusion paths, J. Stat. Phys. 141 (2010) 1071–1092.
[7] R. Friedrich, F. Jenko, A. Baule, S. Eule, Anomalous diffusion of inertial, weakly damped particles, Phys. Rev. Lett. 96 (2006) 230601.
[8] I. Sokolov, R. Metzler, Towards deterministic equations for Levy walks: The fractional material derivative, Phys. Rev. E (2003) 010101.
[9] L. Turgeman, S. Carmi, E. Barkai, Fractional Feynman–Kac equation for non-Brownian functionals, Phys. Rev. Lett. 103 (2009) 190201.
[10] R. Metzler, J. Klafter, The random walk's guide to anomalous diffusion: a fractional dynamics approach, Phy. Rep. 339 (2000) 1–77.
[11] J. Cao, C. Li, Y.Q. Chen, On tempered and substantial fractional calculus, in: 2014 IEEE/ASME 10th International Conference on Mechatronic and Embedded Systems and Applications, MESA, IEEE, 2014, pp. 1–6.
[12] M. Chen, W. Deng, Discretized fractional substantial calculus, ESAIM Math. Model. Numer. 49 (2015) 373–394.
[13] B. Baeumer, M.M. Meerschaert, Tempered stable Lévy motion and transient super-diffusion, J. Comput. Appl. Math. 233 (2010) 2438–2448.
[14] R.G. Buschman, Decomposition of an integral operator by use of Mikusiński calculus, SIAM J. Math. Anal. 3 (1972) 83–85.
[15] A. Cartea, D. del Castillo-Negrete, Fluid limit of the continuous-time random walk with general Levy jump distribution functions, Phys. Rev. E 76 (2007) 041105.
[16] E. Hanert, C. Piret, A Chebyshev pseudospectral method to solve the space–time tempered fractional diffusion equation, SIAM J. Sci. Comput. 36 (2014) A1797–A1812.
[17] A. Kullberg, D. del C -Negrete, Transport in the spatially tempered, fractional Fokker–Planck equation, J. Phys. A 45 (2012) 255101.
[18] M.M. Meerschaert, Y. Zhang, B. Baeumer, Tempered anomalous diffusion in heterogeneous systems, Geophys. Res. Lett. 35 (2008) 190201.
[19] K.B. Oldham, J. Spanier, The Fractional Calculus, Academic Press, New York, London, 1974.
[20] Y. Lin, C. Xu, Finite difference/spectral approximations for the time-fractional diffusion equation, J. Comput. Phys. 225 (2007) 1533–1552.
[21] Z.Z. Sun, X. Wu, A fully discrete difference scheme for a diffusion-wave system, Appl. Numer. Math. 56 (2006) 193–209.
[22] F. Zeng, C. Li, F. Liu, I. Turner, Numerical algorithms for time-fractional subdiffusion equation with second-order accuracy, SIAM J. Sci. Comput. 37 (2015) A55–A78.
[23] A.A. Alikhanov, A new difference scheme for the time fractional diffusion equation, J. Comput. Phys. 280 (2015) 424–438.
[24] G. Gao, H. Sun, Z. Sun, Stability and convergence of finite difference schemes for a class of time-fractional sub-diffusion equations based on certain superconvergence, J. Comput. Phys. 280 (2015) 510–528.
[25] C. Lubich, Discretized fractional calculus, SIAM J. Math. Anal. 17 (1986) 704–719.
[26] W. Deng, M. Chen, E. Barkai, Numerical algorithms for the forward and backward fractional Feynman–Kac equations, J. Sci. Comput. 62 (2015) 718–746.
[27] M. Chen, W. Deng, High order algorithms for the fractional substantial diffusion equation with truncated Lévy flights, SIAM J. Sci. Comput. 37 (2015) A890–A917.
[28] Z.Z. Sun, Numerical Methods of Partial Differential Equations, second ed., Science Press, Beijing, 2012, in Chinese.
[29] W. Cao, Z. Zhang, G.E. Karniadakis, Time-splitting schemes for fractional differential equations I: smooth solutions, SIAM J. Sci. Comput. 37 (4) (2015) A1752–A1776.
[30] W. Cao, F. Zeng, Z. Zhang, G.E. Karniadakis, Implicit-explicit difference schemes for nonlinear fractional differential equations with non-smooth solutions, SIAM J. Sci. Comput. (in press).
[31] B. Jin, R. Lazarov, Z. Zhou, Error estimates for a semidiscrete finite element method for fractional order parabolic equations, SIAM J. Numer. Anal. 51 (2013) 445–466.
[32] F. Zeng, C. Li, F. Liu, I. Turner, The use of finite difference/element approaches for solving the time-fractional subdiffusion equation, SIAM J. Sci. Comput. 35 (2013) A2976–A3000.
[33] I. Podlubny, Fractional Differential Equations, Academic Press, New York, 1999.
[34] C. Tadjeran, M.M. Meerschaert, H.-P. Scheffler, A second-order accurate numerical approximation for the fractional diffusion equation, J. Comput. Phys. 213 (2006) 205–213.
[35] Z.Z. Sun, The Method of Order Reduction and Its Application to the Numerical Solutions of Partial Differential Equations, Science Press, Beijing, 2009.
[36] K. Diethelm, N.J. Ford, A.D. Freed, M. Weilbeer, Pitfalls in fast numerical solvers for fractional differential equations, J. Comput. Appl. Math. 186 (2006) 482–503.
[37] F. Zeng, Z. Zhang, G. Karniadakis, Second-order numerical methods for multi-term fractional differential equations: smooth and non-smooth solutions, SIAM J. Numer. Anal. (submitted for publication).
[38] M. Zayernouri, M. Ainsworth, G. Karniadakis, Tempered fractional Sturm–Liouville eigenproblems, SIAM J. Sci. Comput. 37 (4) (2015) A1777–A1800.