Numerical discretization and error analysis for an optimal control problem governed by forward fractional Feynman-Kac equation*

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Abstract

In this paper, an optimal control problem governed by the forward fractional Feynman-Kac equation is considered, which describes functional distributions of anomalous diffusion and encounters significant challenges arise from the time-space coupled nonlocal operator and its non-commutativity with the Laplacian. First, we investigate the well-posedness of the continuous optimal control problem, derive the first-order optimality conditions and establish the regularity estimates of the solution. Then, the Riemann-Liouville fractional substantial derivative in the equation is approximated by using the backward Euler convolution quadrature formula, and a temporal semi-discrete scheme is proposed for the optimal control problem. Moreover, we rigorously analyze the $\ell^2(L^2(\Omega))$ and $\ell^\infty(L^2(\Omega))$ error estimates of the proposed semi-discrete scheme, which exhibits almost optimal convergence of $O(\tau|\ln\tau|)$, relying only on the regularity assumptions on the data and without extra assumptions on the solution of the optimality system. Finally, we perform the numerical experiments by using the inexact alternating direction method of multipliers (ADMM) algorithm and the piecewise linear finite element method. The numerical results demonstrate the validity of our numerical scheme and verify the theoretical convergence order.

Keywords. optimal control problem, forward fractional Feynman-Kac equation, fractional substantial derivative, convolution quadrature, error estimate

AMS subject classifications. 49K20, 49M25, 35R11, 65M12

1 Introduction

Anomalous diffusion in non-Brownian motion is a widespread phenomenon in various fields, including physics, chemistry, biology, finance and others [9, 21, 22, 26, 27, 28, 34]. The functional of anomalous diffusion has also attracted great interests in the community, see [2, 4, 32] and the references therein. Analogous to Brownian motion, the functional of anomalous diffusion is defined as $\mathbb{A} = \int_0^t V(x(s))ds$, where $x(t)$ is the trajectory of non-Brownian particle and $V(x)$ a prescribed function associated with specific applications [2, 4]. Let $u(x,\mathbb{A},t)$ be the joint probability density function (PDF) of finding the particle on $(x,\mathbb{A})$ at time t, which obeys the power-law waiting time, Carmi et.al in [2, 32] derived that the governing equation of $u(x,\rho,t) := \int_0^\infty u(x,\mathbb{A},t)e^{-\rho\mathbb{A}}d\mathbb{A}$ with positive functional $\mathbb{A}$ is the forward fractional Feynman-Kac equation as follows

$$\partial_t u(x,\rho,t) = \Delta D_t^{1-\alpha,x} u(x,\rho,t) - \rho V(x)u(x,\rho,t), \tag{1.1}$$

which is in Laplace space. $D_t^{1-\alpha,x}$ with $\alpha\in(0,1)$ refers to the left-sided Riemann-Liouville fractional substantial derivative [2, 7, 17], which is defined by

$$D_t^{1-\alpha,x}u(x,\rho,t) = \frac{1}{\Gamma(\alpha)}\left[\partial_t + \rho V(x)\right]\int_0^t (t-s)^{\alpha-1}e^{-(t-s)\rho V(x)}u(x,\rho,s)ds, \tag{1.2}$$

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with $\Gamma(s) = \int_0^\infty t^{s-1}e^{-t}dt$ being the Euler-gamma function, and Δ represents the Laplace operator. If the functional $\mathbb{A}$ is not necessarily positive determined by the function $V(x)$, then $u(x,\rho,t) := \int_{-\infty}^{+\infty} u(x,\mathbb{A},t)e^{-\mathbf{i}\rho\mathbb{A}}\mathrm{d}\mathbb{A}$ refers to the Fourier transform of $u(x,\mathbb{A},t)$, and the corresponding governing equation is a variant of (1.1) with ρ replaced by $-\mathbf{i}\rho$ [2], where $\mathbf{i}$ is the imaginary unit.

It is evident that the operators Δ and $D_t^{1-\alpha,x}$ can not commutate with each other provided that $\rho V(x)$ is not a constant function. If the term $\Delta D_t^{1-\alpha,x}u$ in (1.1) is replaced by $D_t^{1-\alpha,x}\Delta u$, then it corresponds to the backward fractional Feynman-Kac equation [2, 32]

$$\partial_t u(x,\rho,t) = D_t^{1-\alpha,x}\Delta u(x,\rho,t) - \rho V(x)u(x,\rho,t), \tag{1.3}$$

with $u(x,\mathbb{A},t)$ being the PDF of $\mathbb{A}$ at t in the process started at x. For $\alpha = 1$, (1.1) reduces to the classical Feynman-Kac equation describing the functional distribution of normal Brownian motion, which is a Schrödinger-like equation derived by Kac [15] in 1949 by using the Feynman's path integral method. For $\rho V(x) \equiv 0$ and $\alpha \in (0,1)$, $D_t^{1-\alpha,x}$ in (1.1) becomes the Riemann-Liouville derivative $D_t^{1-\alpha}$ defined by (2.5), then it leads to the time-fractional diffusion equation $\partial_t u - \Delta D_t^{1-\alpha}u = 0$ simulating anomalous diffusion phenomena in physics [21, 22, 34].

In this work, we concentrate on an optimal control problem governed by the forward fractional Feynman-Kac equation as follows

$$\min_{q\in U_{ad}} J(u,q) = \frac{1}{2}\|u-u_d\|^2_{L^2(0,T;L^2(\Omega))} + \frac{\gamma}{2}\|q\|^2_{L^2(0,T;L^2(\Omega))}, \tag{1.4}$$

where $u_d : (0,T) \to L^2(\Omega)$ is a given target function, and $\gamma > 0$ is a penalty constant. The state variable u and the control variable q satisfy the forward fractional Feynman-Kac equation

$$\begin{cases} \partial_t u(x,t) - \Delta D_t^{1-\alpha,x}u(x,t) + \rho V(x)u(x,t) = f(x,t) + q(x,t), & (x,t) \in \Omega\times(0,T], \\ u(x,t) = 0, & (x,t) \in \partial\Omega\times(0,T], \\ u(x,0) = 0, & x \in \Omega, \end{cases} \tag{1.5}$$

where $u(x,t) := u(x,\rho,t)$ depends on the complex constant $\rho \in \mathbb{C}$, $f : (0,T] \to L^2(\Omega)$ is a given source term, Ω is a bounded convex polygonal domain in $\mathbb{R}^n$ $(n = 1,2,3)$ with boundary $\partial\Omega$, and the function $V(x)$ is bounded in $\bar{\Omega}$. The control set U_{ad} is given by

$$U_{ad} = \left\{q \in L^2(0,T;L^2(\Omega)) : a \le q \le b \ \text{ a.e. in } \Omega\times[0,T]\right\}, \tag{1.6}$$

with $a, b \in \mathbb{R}$ and $a \le b$.

The numerical investigations of the fractional Feynman-Kac equations are relatively limited, compared with that of subdiffusion equations. The significant challenges on theoretical and numerical analysis come from the time-space coupled nonlocal derivative involved in the governing equation and the non-commutativity of $D_t^{1-\alpha,x}$ and the Laplace operator (i.e., $D_t^{1-\alpha,x}\cdot\Delta \ne \Delta\cdot D_t^{1-\alpha,x}$). In [3], finite difference approximations were established for fractional substantial derivatives based on the Lubich method [20], which were further applied to numerically solving the forward and backward fractional Feynman-Kac equations [5]. In [6], a first-order time-stepping method was provided to solve the forward fractional Feynman-Kac equation (1.1) with error estimates in the measure norm depending only on the measure of the initial data. Recently, [24] built the regularity of the solution for (1.5), and developed the error estimates for a fully discrete scheme constructed by convolution quadrature and finite element method. Some numerical studies for the backward fractional Feynman-Kac equation were also presented in [13, 29, 30].

In the past decade, there exist generous literatures on optimal control problems governed by fractional partial differential equations, both in terms of theoretical issues and numerical algorithms, we can refer to [1, 12, 14, 19, 23, 33, 35, 36] and the references therein. However, to the best of our knowledge, the optimal control problems of the fractional Feynman-Kac equations have not yet been considered in previous works. Compared with the optimal control problems governed by some time-fractional diffusion equations, the problem (1.4)-(1.5) encounters significant challenges in theoretical and numerical analysis due to the time-space coupled nonlocal derivative $D_t^{1-\alpha,x}$ and the non-commutativity of $D_t^{1-\alpha,x}$ and the Laplace operator Δ in (1.5). Moreover, the coupling of the optimality conditions (2.10)-(2.12) reduces the regularity of the solution to the optimal control problem (1.4)-(1.5). To fill this gap, we dedicate to investigating the well-posedness of the optimal control problem (1.4)-(1.5), deriving the first-order optimality conditions and the regularity of its solution with less regularity assumptions on the data. Based on this, a temporal semi-discrete scheme is further proposed and analyzed rigorously. The almost optimal convergence order of $O(\tau|\ln\tau|)$ in time is proved only depending on regularity assumptions on the data without additional regularity requirements on the exact solutions.

The structure of the rest of this paper is as follows. Some preliminaries and essential lemmas are introduced and proved in Section 2, the optimality conditions and the regularity results of the solution to the optimal control problem (1.4)-(1.5) are also derived. In Section 3, we propose a semi-discrete scheme in time for (1.4)-(1.5) by using the backward Euler convolution quadrature formula to approximate the Riemann-Liouville fractional substantial derivative in time. The temporal error estimates both in $\ell^2(L^2(\Omega))$ and $\ell^\infty(L^2(\Omega))$ norms of the proposed semi-discrete scheme are rigorously established in Section 4. In Section 5, some numerical results are provided in order to validate the effectiveness and the theoretical convergence order of our proposed numerical scheme, where the discrete optimal control problem is solved by an inexact ADMM algorithm [8]. We conclude this work with some discussions in the final section.

2 Optimality conditions and regularity

2.1 Preliminaries

Throughout this paper, the notations $(\cdot,\cdot)$ and $\|\cdot\|$ denote the inner product and norm in $L^2(\Omega)$, the latter also stands for the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$. We additionally introduce the Hilbert space $\dot{H}^2(\Omega) = H_0^1(\Omega)\cap H^2(\Omega)$ endowed with the norm $\|\cdot\|_{\dot{H}^2(\Omega)} := \|\Delta\cdot\|$ in [31], where $H^2(\Omega) = W^{2,2}(\Omega)$ is the standard Sobolev space.

By [17, Proposition 7], the Laplace transform of the left-sided Riemann-Liouville fractional substantial derivative with $\alpha \in (0,1)$ and $u(x,0) = 0$ is

$$\widehat{D_t^{1-\alpha,x}u}(\xi) = \beta(\xi)^{1-\alpha}\hat{u}(\xi), \tag{2.1}$$

where '$\widehat{\ }$' means taking the Laplace transform and

$$\beta(\xi) := \xi + \rho V(x). \tag{2.2}$$

In the following, we introduce two essential lemmas for establishing the regularity results for the solutions.

Lemma 2.1 ([10]). *For any $\xi \in \Sigma_\theta := \left\{\xi \in \mathbb{C}\backslash\{0\} : |\arg\xi| \le \theta < \pi\right\}$ with $\theta \in (0,\pi)$, we have the resolvent estimates*

$$\|(\xi-\Delta)^{-1}\| \le C|\xi|^{-1}, \tag{2.3}$$

$$\|\Delta^{1-\gamma}(\xi-\Delta)^{-1}\| \le C|\xi|^{-\gamma},\ \gamma \in [0,1]. \tag{2.4}$$

Lemma 2.2 ([6]). *Let $\beta(\xi)$ be defined in (2.2) and $V(x)$ bounded in $\bar{\Omega}$. By choosing $\theta \in (\frac{\pi}{2},\pi)$ sufficiently close to $\frac{\pi}{2}$ and $\kappa > 0$ sufficiently large (depending on $|\rho|\|V(x)\|_{L^\infty(\bar{\Omega})}$), we have the following results.*

(1) For all $x \in \Omega$ and $\xi \in \Sigma_{\theta,\kappa} := \{\xi \in \mathbb{C} : |\xi| \ge \kappa, |\arg\xi| \le \theta\}$, it holds that $\beta(\xi) \in \Sigma_{\frac{3\pi}{4},\frac{\kappa}{2}}$ and

$$C_1|\xi| \le |\beta(\xi)| \le C_2|\xi|,$$

where C_1, C_2 are positive constants. Thus $\beta(\xi)^{1-\alpha}$ and $\beta(\xi)^{\alpha-1}$ are both $C(\bar{\Omega})$ valued analytic function of $\xi \in \Sigma_{\theta,\kappa}$.

(2) The operator $(\beta(\xi)^\alpha - \Delta)^{-1} : L^2(\Omega) \to L^2(\Omega)$ is well-defined, bounded, and analytic for $z \in \Sigma_{\theta,\kappa}$, satisfying

$$
\begin{aligned}
&\|(\beta(\xi)^\alpha - \Delta)^{-1}\| \le C|\xi|^{-\alpha}, \quad \forall\, \xi \in \Sigma_{\theta,\kappa},\\
&\|\Delta(\beta(\xi)^\alpha - \Delta)^{-1}\| \le C, \qquad \forall\, \xi \in \Sigma_{\theta,\kappa}.
\end{aligned}
$$

The left-sided Riemann-Liouville fractional derivative [25] is defined by

$$
D_t^{1-\alpha} u(x,t) = \frac{1}{\Gamma(\alpha)} \partial_t \int_0^t (t-s)^{\alpha-1} u(x,s) ds, \quad \alpha \in (0,1), \tag{2.5}
$$

and ${}^B D_t^{1-\alpha}$ denotes the right-sided Riemann-Liouville fractional derivative [25] by

$$
{}^B D_t^{1-\alpha} z(x,t) = -\frac{1}{\Gamma(\alpha)} \partial_t \int_t^T (s-t)^{\alpha-1} z(x,s) \mathrm{d}s, \quad \alpha \in (0,1).
$$

It is indicated in [18, Lemma 2.3] that the left- and right-sided Riemann-Liouville fractional derivatives satisfy the fractional integration by parts formula, that is

$$
\int_0^T D_t^{1-\alpha} u(x,t) \cdot z(x,t) \mathrm{d}t = \int_0^T u(x,t) \cdot {}^B D_t^{1-\alpha} z(x,t) \mathrm{d}t, \tag{2.6}
$$

and we can also derive the similar result for the fractional substantial derivative given by (1.2) in the following lemma.

Lemma 2.3. *For $\alpha \in (0,1)$, we have*

$$
\int_0^T D_t^{1-\alpha,x} u(x,t) \cdot z(x,t) \mathrm{d}t = \int_0^T u(x,t) \cdot {}^B D_t^{1-\alpha,x} z(x,t) \mathrm{d}t, \tag{2.7}
$$

where ${}^B D_t^{1-\alpha,x}$ is the adjoint operator of $D_t^{1-\alpha,x}$, and given by

$$
{}^B D_t^{1-\alpha,x} z(x,t) = e^{t\rho V(x)} {}^B D_t^{1-\alpha} \big(e^{-t\rho V(x)} z(x,t)\big). \tag{2.8}
$$

Proof. As mentioned in [17], the fractional substantial derivative (1.2) satisfies

$$
D_t^{1-\alpha,x} u(x,t) = e^{-t\rho V(x)} D_t^{1-\alpha} \big(e^{t\rho V(x)} u(x,t)\big). \tag{2.9}
$$

Then we have from (2.6) that

$$
\begin{aligned}
\int_0^T D_t^{1-\alpha,x} u(x,t) \cdot z(x,t) \mathrm{d}t &= \int_0^T e^{-t\rho V(x)} D_t^{1-\alpha} \big(e^{t\rho V(x)} u(x,t)\big) \cdot z(x,t) \mathrm{d}t \\
&= \int_0^T e^{t\rho V(x)} u(x,t) \cdot {}^B D_t^{1-\alpha} \big(e^{-t\rho V(x)} z(x,t)\big) \mathrm{d}t \\
&= \int_0^T u(x,t) \cdot {}^B D_t^{1-\alpha,x} z(x,t) \mathrm{d}t,
\end{aligned}
$$

which completes the proof. □

2.2 Optimality conditions

In this subsection, the well-posedness of the continuous optimal control problem (1.4)-(1.5) and the first-order optimality conditions are established.

Theorem 2.4. *Let $q \in U_{ad}$ be the solution to the optimal control problem (1.4)-(1.5), and $u \in L^2(0,T;L^2(\Omega))$ the corresponding state variable determined by (1.5). Then there exists an adjoint state $z \in L^2(0,T;L^2(\Omega))$ such that (u,z,q) satisfies the following optimality conditions*

$$\partial_t u - \Delta D_t^{1-\alpha,x} u + \rho V(x) u = f + q, \ \text{in } \Omega \times (0,T], \ \ u = 0, \ \text{on } \partial\Omega \times (0,T], \tag{2.10}$$

$$-\partial_t z - {}^B D_t^{1-\alpha,x} \Delta z + \rho V(x) z = u - u_d, \ \text{in } \Omega \times [0,T), \ \ z = 0, \ \text{on } \partial\Omega \times [0,T), \tag{2.11}$$

with $u(\cdot,0) = 0$, $z(\cdot,T) = 0$, and the variational inequality

$$J'(q)(v-q) = \int_0^T \int_\Omega (\gamma q + z)(v-q) \mathrm{d}x\mathrm{d}t \geq 0, \ \ \forall\, v \in U_{ad}. \tag{2.12}$$

Proof. Let $J(q) := J(u(q),q)$. The first-order necessary optimality condition of the optimal control problem (1.4)-(1.5) reads

$$J'(q)(v-q) = \int_0^T \int_\Omega (u-u_d)\delta u(q) \mathrm{d}x\mathrm{d}t + \int_0^T \int_\Omega \gamma q(v-q) \mathrm{d}x\mathrm{d}t \geq 0, \ \ \forall\, v \in U_{ad},$$

where $\delta u(q) = \lim_{\epsilon \to 0}[u(q+\epsilon(v-q)) - u(q)]/\epsilon$, it satisfies zero boundary and initial values, and

$$\partial_t \delta u(q) - \Delta D_t^{1-\alpha,x} \delta u(q) + \rho V(x) \delta u(q) = v - q. \tag{2.13}$$

Then we obtain from the adjoint equation (2.11), the perturbation equation (2.13) and the property (2.7) in Lemma 2.3 that

$$\begin{aligned} \int_0^T \int_\Omega (u-u_d)\delta u(q) \mathrm{d}x\mathrm{d}t &= \int_0^T \int_\Omega \big(-\partial_t z - {}^B D_t^{1-\alpha,x} \Delta z + \rho V(x) z \big) \delta u(q) \mathrm{d}x\mathrm{d}t \\ &= \int_0^T \int_\Omega z \big(\partial_t \delta u(q) - \Delta D_t^{1-\alpha,x} \delta u(q) + \rho V(x) \delta u(q) \big) \mathrm{d}x\mathrm{d}t \\ &= \int_0^T \int_\Omega z(v-q) \mathrm{d}x\mathrm{d}t, \end{aligned}$$

which implies the variational inequality (2.12). □

From Theorem 2.4, it deduces that the objective functional $J(\cdot)$ in (1.4) is strongly convex with respect to the control variable q, and

$$J'(p)(p-q) - J'(q)(p-q) \geq \gamma \|p-q\|^2_{L^2(0,T;L^2(\Omega))} \tag{2.14}$$

for any $p, q \in L^2(0,T;L^2(\Omega))$. Then the continuous optimal control problem (1.4)-(1.5) has a unique solution. The variational inequality (2.12) yields that

$$q = P_{U_{ad}}\Big(-\frac{1}{\gamma} z \Big), \tag{2.15}$$

where $P_{U_{ad}}(\cdot)$ denotes the pointwise projection onto the admissible set U_{ad}, denoted by

$$P_{U_{ad}}\big(v(t)\big) = \max\big\{a, \min\{v(t), b\}\big\}. \tag{2.16}$$

As stated in [16, Corollary 2.4], the projection $P_{U_{ad}}(\cdot)$ is nonexpansive, i.e.,

$$\|P_{U_{ad}}(v) - P_{U_{ad}}(w)\|_{H^1(0,T;L^2(\Omega))} \leq \|v-w\|_{H^1(0,T;L^2(\Omega))}, \ \ \forall\, v, w \in H^1(0,T;L^2(\Omega)),$$

which implies the following estimate

$$\|P_{U_{ad}}(v)\|_{H^1(0,T;L^2(\Omega))} \leq \|v\|_{H^1(0,T;L^2(\Omega))} + C, \ \ \forall\, v \in H^1(0,T;L^2(\Omega)). \tag{2.17}$$

2.3 Solution representations and regularity

In this subsection, we present the integral representations of the solutions to the optimality system (2.10)-(2.12), and establish the corresponding regularity results.

Lemma 2.5. *The solutions to the state and adjoint equations* (2.10)-(2.11) *are represented by*

$$u(\cdot,t)=\int_0^t E(t-s)\big(f(\cdot,s)+q(\cdot,s)\big)\mathrm{d}s, \tag{2.18}$$

$$z(\cdot,t)=\int_t^T F(s-t)\big(u(\cdot,s)-u_d(\cdot,s)\big)\mathrm{d}s, \tag{2.19}$$

respectively, where the operators $E(\cdot)$ *and* $F(\cdot)$ *mapping from* $L^2(\Omega)$ *to* $L^2(\Omega)$ *are given by*

$$E(t)v:=\frac{1}{2\pi\mathbf{i}}\int_{\Gamma_{\theta,\kappa}} e^{\xi t}\beta(\xi)^{\alpha-1}\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}v\mathrm{d}\xi,\ \ \forall\, v\in L^2(\Omega), \tag{2.20}$$

$$F(t)v:=\frac{1}{2\pi\mathbf{i}}\int_{\Gamma_{\theta,\kappa}} e^{\xi t}\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}\beta(\xi)^{\alpha-1}v\mathrm{d}\xi,\ \ \forall\, v\in L^2(\Omega), \tag{2.21}$$

$\beta(\xi)$ *is given by* (2.2)*, and* $\Gamma_{\theta,\kappa}$ *refers to*

$$\Gamma_{\theta,\kappa}=\big\{z\in\mathbb{C}:|z|=\kappa,|\arg z|\le\theta\big\}\cup\big\{z\in\mathbb{C}:|z|\ge\kappa,\ |\arg z|=\theta\big\}.$$

Note that $\beta(\xi)^{\alpha-1}\cdot\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}\neq\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}\cdot\beta(\xi)^{\alpha-1}$ *if* $\rho V(x)$ *is not a constant function, thus the operator* $E(\cdot)$ *significantly differs from* $F(\cdot)$.

Proof. We first consider to derive (2.18). By (2.1) and taking the Laplace transform of (2.10), it yields that

$$\hat{u}(\xi)=\beta(\xi)^{\alpha-1}\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}\big(\hat{f}(\xi)+\hat{q}(\xi)\big). \tag{2.22}$$

Then by the rule of inverse Laplace transform $\mathcal{L}^{-1}(\hat{f}\hat{g})(t)=\int_0^t\mathcal{L}^{-1}(\hat{f})(t-s)\mathcal{L}^{-1}(\hat{g})(s)\mathrm{d}s$ and the definition of $E(\cdot)$ in (2.20), we obtain (2.18) by utilizing Cauchy's integral formula and theorem.

Let $\eta=T-t$, $p(\cdot,\eta):=z(\cdot,T-\eta)=z(\cdot,t)$, $\bar{u}(\cdot,\eta)=u(\cdot,T-\eta)=u(\cdot,t)$ and $\bar{u}_d(\cdot,\eta)=u_d(\cdot,T-\eta)=u_d(\cdot,t)$. By (2.8), (2.9) and variable changing, we have

$$-\partial_t z(t)=\partial_\eta p(\eta),\ \ {}^{B}D_t^{1-\alpha,x}\Delta z(t)=D_\eta^{1-\alpha,x}\Delta p(\eta).$$

Then the adjoint equation (2.11) becomes

$$\partial_\eta p(\eta)-D_\eta^{1-\alpha,x}\Delta p(\eta)+\rho V(x)p(\eta)=(\bar{u}-\bar{u}_d)(\eta),\ \ \eta\in(0,T],\ \ \text{with}\ \ p(0)=0.$$

Hence, by the approach of Laplace transform, it follows that

$$p(\eta)=\int_0^\eta F(\eta-r)(\bar{u}-\bar{u}_d)(r)\mathrm{d}r,$$

which leads to (2.19) by setting $r=T-s$ and $\eta=T-t$. □

Lemma 2.6. *Let* $V(x)\in W^{2,\infty}(\Omega)$*. The operators* $E(\cdot)$ *and* $F(\cdot)$ *given by* (2.20) *and* (2.21) *satisfy the following estimates*

$$\|E(t)\|\le C,\quad \|\Delta E(t)\|\le Ct^{-\alpha}, \tag{2.23}$$

$$\|F(t)\|\le C,\quad \|\Delta F(t)\|\le Ct^{-\alpha}. \tag{2.24}$$

Proof. The estimates $\|E(t)\| \le C$, $\|F(t)\| \le C$ and $\|\Delta F(t)\| \le Ct^{-\alpha}$ can be easily obtained from (2.20) and (2.21) by using Lemma 2.2.

Next, we consider the estimate for $\|\Delta E(t)\|$. As $V(x) \in W^{2,\infty}(\Omega)$, it follows from Lemma 2.2 and [31, Lemma 3.1] that

$$\begin{aligned}\|\beta(\xi)^{\alpha-1}v\|_{\dot{H}^2(\Omega)} &= \|\Delta(\beta(\xi)^{\alpha-1}v)\| \\ &\le \|(\Delta\beta(\xi)^{\alpha-1})v\| + 2\|\nabla(\beta(\xi)^{\alpha-1})\cdot\nabla v\| + \|\beta(\xi)^{\alpha-1}\Delta v\| \\ &\le C|\xi|^{\alpha-1}\|v\|_{\dot{H}^2(\Omega)}, \quad \forall\, \xi \in \Gamma_{\theta,\kappa},\end{aligned}$$

where $|\xi| \ge \kappa$ is applied. Then we have from Lemma 2.2 that

$$\begin{aligned}&\|\beta(\xi)^{\alpha-1}\|_{\dot{H}^2(\Omega)\to\dot{H}^2(\Omega)} \le C|\xi|^{\alpha-1}, \\ &\big\|\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}\big\|_{L^2(\Omega)\to\dot{H}^2(\Omega)} \le \big\|\Delta\big(\beta(\xi)^{\alpha}-\Delta\big)^{-1}\big\| \le C,\end{aligned}$$

which implies that $\|\Delta E(t)\| \le Ct^{-\alpha}$. □

Now, we start to analyze the regularity of the solutions to the optimality conditions (2.10)-(2.12), the results are stated in the following theorem.

Theorem 2.7. *Let (u, z, q) be the solutions to the system (2.10)-(2.12). Suppose that $f, u_d \in L^2(0,T;L^2(\Omega))$, $V(x) \in W^{2,\infty}(\Omega)$ and the real part $\mathrm{Re}(\rho V(x)) \ge 0$. Then we have*

$$\|u\|_{H^1(0,T;L^2(\Omega))} + \|u\|_{L^2(0,T;\dot{H}^2(\Omega))} \le C\|f+q\|_{L^2(0,T;L^2(\Omega))}, \tag{2.25}$$

$$\|z\|_{H^1(0,T;L^2(\Omega))} + \|z\|_{L^2(0,T;\dot{H}^2(\Omega))} \le C\|u-u_d\|_{L^2(0,T;L^2(\Omega))}, \tag{2.26}$$

$$\|q\|_{H^1(0,T;L^2(\Omega))} \le C\|u-u_d\|_{L^2(0,T;L^2(\Omega))} + C. \tag{2.27}$$

Proof. By (2.23) in Lemma 2.6, we can easily obtain the estimate of u in (2.18) that

$$\|u(t)\|_{L^2(\Omega)} \le C\int_0^t \|(f+q)(s)\|\mathrm{d}s, \tag{2.28}$$

which implies $\|u\|_{L^2(0,T;L^2(\Omega))} \le C\|f+q\|_{L^2(0,T;L^2(\Omega))}$. In addition, it also follows from (2.23) in Lemma 2.6 that

$$\|u(t)\|_{\dot{H}^2(\Omega)} \le C\int_0^t (t-s)^{-\alpha}\|(f+q)(s)\|_{L^2(\Omega)}\mathrm{d}s.$$

Then we have from Young's inequality for convolution that

$$\|u\|_{L^2(0,T;\dot{H}^2(\Omega))} \le C\|f+q\|_{L^2(0,T;L^2(\Omega))}.$$

Similarly, we can derive from (2.19), (2.21) and Lemma 2.2 that

$$\|z\|_{L^2(0,T;L^2(\Omega))} + \|z\|_{L^2(0,T;\dot{H}^2(\Omega))} \le C\|u-u_d\|_{L^2(0,T;L^2(\Omega))}. \tag{2.29}$$

Next, it remains to derive the estimate $\|u\|_{H^1(0,T;L^2(\Omega))} \le C\|f+q\|_{L^2(0,T;L^2(\Omega))}$. We extend u to be zero for $t < 0$ and f, q to be zero for $t \in \mathbb{R}\backslash[0,T]$. Let $\mathcal{F}$ and $\mathcal{L}$ denote the Fourier and Laplace transforms, respectively, it holds $\mathcal{F}v(\omega) = \mathcal{L}v(\xi)$ with $\xi = \mathbf{i}\omega$ and $\omega \in \mathbb{R}$. Then it follows from (2.22) that

$$\begin{aligned}(\partial_t + \rho V(x))u &= \mathcal{L}^{-1}\big\{\beta(\xi)\mathcal{L}u(\xi)\big\}(t) \\ &= \mathcal{F}^{-1}\big\{(\mathbf{i}\omega+\rho V(x))^{\alpha}\big((\mathbf{i}\omega+\rho V(x))^{\alpha}-\Delta\big)^{-1}\mathcal{F}(f+q)(\omega)\big\}(t).\end{aligned}$$

Let $\rho = a + b\mathbf{i}$, it has $\mathbf{i}\omega + \rho V(x) = aV(x) + \mathbf{i}(\omega + bV(x))$, then $|\arg(\mathbf{i}\omega+\rho V(x))^{\alpha}| \le \frac{\pi}{2}$ due to $aV(x) = \mathrm{Re}(\rho V(x)) \ge 0$. Then we have from Lemma 2.1 and the Plancherel formula that

$$\|(\partial_t + \rho V(x))u\|_{L^2(0,T;L^2(\Omega))} \le \|(\partial_t + \rho V(x))u\|_{L^2(\mathbb{R};L^2(\Omega))}$$

$$
\begin{aligned}
&= \left\|\mathcal{F}^{-1}\{(\mathbf{i}\omega+\rho V(x))^{\alpha}\big((\mathbf{i}\omega+\rho V(x))^{\alpha}-\Delta\big)^{-1}\mathcal{F}(f+q)\}\right\|_{L^2(\mathbb{R};L^2(\Omega))}\\
&= \left\|(\mathbf{i}\omega+\rho V(x))^{\alpha}\big((\mathbf{i}\omega+\rho V(x))^{\alpha}-\Delta\big)^{-1}\mathcal{F}(f+q)\right\|_{L^2(\mathbb{R};L^2(\Omega))}\\
&\le C\|\mathcal{F}(f+q)\|_{L^2(\mathbb{R};L^2(\Omega))}\\
&= C\|f+q\|_{L^2(\mathbb{R};L^2(\Omega))}\\
&= C\|f+q\|_{L^2(0,T;L^2(\Omega))}.
\end{aligned}
$$

Further, it holds that

$$
\begin{aligned}
\|\partial_t u\|_{L^2(0,T;L^2(\Omega))} &\le \|(\partial_t+\rho V(x))u\|_{L^2(0,T;L^2(\Omega))}+\|\rho V(x)u\|_{L^2(0,T;L^2(\Omega))}\\
&\le C\|f+q\|_{L^2(0,T;L^2(\Omega))}+C\|u\|_{L^2(0,T;L^2(\Omega))}\\
&\le C\|f+q\|_{L^2(0,T;L^2(\Omega))}.
\end{aligned}
$$

Thus, we obtain the estimate (2.25). By the similar approach, (2.26) can also be derived. Finally, (2.27) is deduced from (2.15) and (2.17). □

3 Temporal semi-discrete scheme

In this section, we propose a temporal semi-discrete scheme for solving the optimal control problem (1.4)-(1.5) by using the backward Euler convolution quadrature to approximate the Riemann-Liouville fractional substantial derivative, then derive the corresponding optimality conditions and the representations of the discrete solutions.

We divide the time interval $[0,T]$ into a uniform partition with a step size $\tau = T/N$, i.e., $t_n = n\tau,\ n = 0,1,\cdots,N$. The Riemann-Liouville fractional substantial derivative $D_t^{1-\alpha,x}u(x,t_n)$ can be approximated [3, 6, 29] by

$$
\bar{D}_\tau^{1-\alpha,x}U^n = \frac{1}{\tau^{1-\alpha}}\sum_{j=1}^{n} b_{n-j}^{(1-\alpha)} e^{-t_{n-j}\rho V(x)}U^j,\quad n=1,2,\cdots,N, \tag{3.1}
$$

where the coefficients $\{b_j^{(1-\alpha)}\}$ are determined by the recursive formula $b_0 = 1,\ b_j = b_{j-1}\cdot\frac{\alpha+j-2}{j},\ j = 1,2,\cdots$, and satisfy the power series expansion:

$$
\big(\delta_\tau(\zeta)\big)^{1-\alpha} = \frac{1}{\tau^{1-\alpha}}\sum_{j=0}^{\infty} b_j^{(1-\alpha)}\zeta^j,\ \ \forall\,|\zeta|<1,\ \zeta\in\mathbb{C},\quad \delta_\tau(\zeta)=\frac{1-\zeta}{\tau}. \tag{3.2}
$$

As $\partial_t u + \rho V(x)u = e^{-t\rho V(x)}\partial_t(e^{t\rho V(x)}u)$, we approximate it by

$$
\bar{D}_\tau^{1,x}U^n := e^{-t_n\rho V(x)}\bar{D}_\tau(e^{t_n\rho V(x)}U^n) = \frac{U^n - e^{-\tau\rho V(x)}U^{n-1}}{\tau}, \tag{3.3}
$$

where $\bar{D}_\tau$ denotes the standard backward Euler difference operator $\bar{D}_\tau U^n := \frac{U^n-U^{n-1}}{\tau}$. Then we propose a temporal semi-discrete scheme for the optimal control problem (1.4)-(1.5) as follows

$$
\min_{\mathbf{Q}\in U_{ad}^\tau} J(\mathbf{Q}) = \frac{\tau}{2}\sum_{n=1}^{N}\left(\|U^n-u_d^n\|^2+\gamma\|Q^{n-1}\|^2\right) \tag{3.4}
$$

subject to

$$
\begin{cases}
\bar{D}_\tau^{1,x}U^n - \Delta\bar{D}_\tau^{1-\alpha,x}U^n = f^n + Q^{n-1},\ \ x\in\Omega,\ \ n=1,2,\cdots,N,\\
U^0 = 0,\ \ x\in\Omega,\ \ \text{and}\ \ U^n=0,\ \ x\in\partial\Omega,\ \ n=0,1,\cdots,N,
\end{cases} \tag{3.5}
$$

where $f^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} f(\cdot,t)\mathrm{d}t$, $u_d^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} u_d(\cdot,t)\mathrm{d}t$, and

$$
U_{ad}^\tau = \left\{\mathbf{Q} = \left(Q^{n-1}\right)_{n=1}^{N} : a \le Q^{n-1} \le b,\ n=1,2,\cdots,N\right\}.
$$

3.1 Optimality conditions

In this subsection, we derive the optimality conditions of the temporal semi-discrete problem (3.4)-(3.5).

The adjoint operations of those in (3.1) and (3.3), denoted by ${}^{B}\bar{D}_{\tau}^{1-\alpha,x}Z^{n-1}$ and ${}^{B}\bar{D}_{\tau}^{1,x}Z^{n-1}$, respectively, can be regarded as the temporal difference approximations of ${}^{B}D_{t}^{1-\alpha,x}z(x,t_{n-1})$ and $(-\partial_t+\rho V(x))z(x,t_{n-1})$, and given by

$$ {}^{B}\bar{D}_{\tau}^{1-\alpha,x}Z^{n-1} := \frac{1}{\tau^{1-\alpha}}\sum_{j=n}^{N} b_{j-n}^{(1-\alpha)} e^{-t_{j-n}\rho V(x)} Z^{j-1}, \tag{3.6} $$

$$ {}^{B}\bar{D}_{\tau}^{1,x}Z^{n-1} := e^{t_{n-1}\rho V(x)}\,{}^{B}\bar{D}_{\tau}(e^{-t_{n-1}\rho V(x)}Z^{n-1}) = \frac{Z^{n-1}-e^{-\tau\rho V(x)}Z^{n}}{\tau}, \tag{3.7} $$

with ${}^{B}\bar{D}_{\tau}Z^{n-1} := \frac{Z^{n-1}-Z^{n}}{\tau}$. By using the above definitions and after simple calculations, we can obtain the following equalities:

$$ \begin{aligned} \tau\sum_{n=1}^{N}(Z^{n-1},\bar{D}_{\tau}^{1-\alpha,x}U^{n}) &= \tau\sum_{n=1}^{N}\Big(Z^{n-1},\frac{1}{\tau^{1-\alpha}}\sum_{j=1}^{n} b_{n-j}^{(1-\alpha)} e^{-t_{n-j}\rho V(x)}U^{j}\Big) \\ &= \tau\sum_{j=1}^{N}\sum_{n=j}^{N}\Big(\frac{1}{\tau^{1-\alpha}} b_{n-j}^{(1-\alpha)} e^{-t_{n-j}\rho V(x)}Z^{n-1},U^{j}\Big) \\ &= \tau\sum_{n=1}^{N}\Big(\frac{1}{\tau^{1-\alpha}}\sum_{j=n}^{N} b_{j-n}^{(1-\alpha)} e^{-t_{j-n}\rho V(x)}Z^{j-1},U^{n}\Big) \\ &= \tau\sum_{n=1}^{N}({}^{B}\bar{D}_{\tau}^{1-\alpha,x}Z^{n-1},U^{n}), \end{aligned} \tag{3.8} $$

$$ \begin{aligned} \tau\sum_{n=1}^{N}(Z^{n-1},\bar{D}_{\tau}^{1,x}U^{n}) &= \tau\sum_{n=1}^{N}\Big(Z^{n-1},\frac{U^{n}-e^{-\tau\rho V(x)}U^{n-1}}{\tau}\Big) \\ &= \tau\sum_{n=1}^{N}\Big(Z^{n-1},\frac{U^{n}}{\tau}\Big) - \tau\sum_{n=1}^{N}\Big(Z^{n},\frac{e^{-\tau\rho V(x)}U^{n}}{\tau}\Big) \\ &= \tau\sum_{n=1}^{N}\Big(\frac{Z^{n-1}-e^{-\tau\rho V(x)}Z^{n}}{\tau},U^{n}\Big) \\ &= \tau\sum_{n=1}^{N}({}^{B}\bar{D}_{\tau}^{1,x}Z^{n-1},U^{n}), \end{aligned} \tag{3.9} $$

where $U^0=0$ and $Z^N=0$ are applied. Furthermore, we denote

$$ \mathbf{U}=(U^n)_{n=1}^{N},\quad \mathbf{Z}=(Z^{n-1})_{n=1}^{N},\quad \mathbf{Q}=(Q^{n-1})_{n=1}^{N}. \tag{3.10} $$

Theorem 3.1. *The temporal semi-discrete problem (3.4)-(3.5) admits a unique solution $(\mathbf{U},\mathbf{Q})$ and an adjoint state $\mathbf{Z}$ such that $(\mathbf{U},\mathbf{Z},\mathbf{Q})$ satisfies the optimality system*

$$ \bar{D}_{\tau}^{1,x}U^{n} - \Delta\bar{D}_{\tau}^{1-\alpha,x}U^{n} = f^{n}+Q^{n-1}, \qquad x\in\Omega,\ \ U^{n}=0,\ x\in\partial\Omega, \tag{3.11} $$

$$ {}^{B}\bar{D}_{\tau}^{1,x}Z^{n-1} - {}^{B}\bar{D}_{\tau}^{1-\alpha,x}\Delta Z^{n-1} = U^{n}-u_{d}^{n},\ \ x\in\Omega,\ \ Z^{n-1}=0,\ x\in\partial\Omega, \tag{3.12} $$

for $n=1,2,\cdots,N$ with $U^0=0$, $Z^N=0$, and the variational inequality

$$ (\gamma Q^{n-1}+Z^{n-1}, v-Q^{n-1}) \geq 0,\ \ \forall\, v\in L^2(\Omega),\ a\leq v\leq b. \tag{3.13} $$

Moreover, the variational inequality further yields

$$ Q^{n-1} = P_{U_{ad}}\big(-\frac{1}{\gamma}Z^{n-1}\big). \tag{3.14} $$

Proof. The temporal semi-discrete problem (3.4)-(3.5) has a unique solution $(\mathbf{U},\mathbf{Q})$ due to the strong convexity of the functional $J(\cdot)$ in (3.4). Next, we derive the first-order necessary optimality conditions.

For any $\mathbf{v}\in U_{ad}^{\tau}$ and $\delta\mathbf{Q}:=\mathbf{v}-\mathbf{Q}$, the convexity of U_{ad}^{τ} shows $\mathbf{Q}+\epsilon\delta\mathbf{Q}\in U_{ad}^{\tau}$ for $0<\epsilon\ll 1$. Since $\mathbf{Q}$ is the minimizer of the problem (3.4)-(3.5), then we have

$$J'(\mathbf{Q})\delta\mathbf{Q}=\tau\sum_{n=1}^{N}\int_{\Omega}(U^n-u_d^n)\delta U^n\mathrm{d}x+\tau\sum_{n=1}^{N}\int_{\Omega}\gamma Q^{n-1}\delta Q^{n-1}\mathrm{d}x\geq 0,$$

where $\delta U^n=\lim_{\epsilon\to 0}\big(U^n(Q^{n-1}+\epsilon\delta Q^{n-1})-U^n(Q^{n-1})\big)/\epsilon$ satisfies

$$\bar{D}_{\tau}^{1,x}\delta U^n-\Delta\bar{D}_{\tau}^{1-\alpha,x}\delta U^n=\delta Q^{n-1}.$$

Hence, multiplying δU^n on both sides of (3.12) and summing up yield that

$$\tau\sum_{n=1}^{N}\int_{\Omega}(U^n-u_d^n)\delta U^n\mathrm{d}x=\tau\sum_{n=1}^{N}\int_{\Omega}Z^{n-1}\delta Q^{n-1}\mathrm{d}x,$$

where (3.8) and (3.9) are applied, thus it further derives (3.13). □

3.2 Solution representations

In this subsection, we derive the solution representations for the temporal semi-discrete scheme (3.11)-(3.12) and establish the corresponding stability results.

Lemma 3.2. *Let U^n, Z^{n-1} be the solutions to the temporal semi-discrete scheme (3.11)-(3.12), and define*

$$f_{\tau}(\cdot,t)|_{(t_{n-1},t_n]}=f^n,\quad Q(\cdot,t)|_{[t_{n-1},t_n)}=Q^{n-1},\quad n=1,2,\cdots,N, \tag{3.15}$$
$$U(\cdot,t)|_{(t_{n-1},t_n]}=U^n,\quad u_{d\tau}(\cdot,t)|_{(t_{n-1},t_n]}=u_d^n,\quad n=1,2,\cdots,N. \tag{3.16}$$

Then we have

$$U^n=\int_0^{t_n}E^{\tau}(t_n-s)\big(f_{\tau}(\cdot,s)+Q(\cdot,s)\big)\mathrm{d}s, \tag{3.17}$$
$$Z^{n-1}=\int_{t_{n-1}}^{T}F^{\tau}(s-t_{n-1})\big(U(\cdot,s)-u_{d\tau}(\cdot,s)\big)\mathrm{d}s, \tag{3.18}$$

and

$$E^{\tau}(t)v=\frac{1}{2\pi\mathbf{i}}\int_{\Gamma_{\theta,\kappa}^{\tau}}e^{\xi t}\frac{\xi\tau}{e^{\xi\tau}-1}\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha-1}\big(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha}-\Delta\big)^{-1}v\mathrm{d}\xi, \tag{3.19}$$
$$F^{\tau}(t)v=\frac{1}{2\pi\mathbf{i}}\int_{\Gamma_{\theta,\kappa}^{\tau}}e^{\xi t}\frac{\xi\tau}{e^{\xi\tau}-1}\big(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha}-\Delta\big)^{-1}\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha-1}v\mathrm{d}\xi, \tag{3.20}$$

where $\Gamma_{\theta,\kappa}^{\tau}$ is given by

$$\Gamma_{\theta,\kappa}^{\tau}=\big\{z\in\mathbb{C}:|z|=\kappa,\ |\arg z|\leq\theta\big\}\cup\big\{z\in\mathbb{C}:\kappa\leq|z|\leq\frac{\pi}{\tau\sin\theta},\ |\arg z|=\theta\big\}.$$

Note that if $\rho V(x)\neq C$, then

$$\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha-1}\cdot\big(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha}-\Delta\big)^{-1}\neq\big(\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha}-\Delta\big)^{-1}\cdot\delta_{\tau}(e^{-\tau\beta(\xi)})^{\alpha-1},$$

it indicates that the operator $E^{\tau}(t)$ is essentially different from $F^{\tau}(t)$.

Proof. By (3.1) and (3.3), we can obtain that

$$\sum_{n=1}^{\infty}(\bar{D}_{\tau}^{1-\alpha,x}U^n)\zeta^n = \delta_\tau(e^{-\tau\rho V(x)}\zeta)^{1-\alpha}\sum_{n=1}^{\infty}U^n\zeta^n,$$
$$\sum_{n=1}^{\infty}(\bar{D}_{\tau}^{1,x}U^n)\zeta^n = \delta_\tau(e^{-\tau\rho V(x)}\zeta)\sum_{n=1}^{\infty}U^n\zeta^n.$$

Let $\tilde{U}(\zeta) = \sum_{n=1}^{\infty}U^n\zeta^n$, multiplying (3.11) by ζ^n and summing n from 1 to ∞ yield that

$$\tilde{U}(\zeta) = \delta_\tau(e^{-\tau\rho V(x)}\zeta)^{\alpha-1}\big(\delta_\tau(e^{-\tau\rho V(x)}\zeta)^{\alpha}-\Delta\big)^{-1}\sum_{n=1}^{\infty}(f^n+Q^{n-1})\zeta^n.$$

Using Cauchy's integral formula and theorem, we derive that

$$U^n = \frac{\tau}{2\pi\mathbf{i}}\int_{\Gamma_{\theta,\kappa}^{\tau}} e^{\xi t_n}\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\big(\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha}-\Delta\big)^{-1}\sum_{n=1}^{\infty}(f^n+Q^{n-1})e^{-\xi t_n}\mathrm{d}\xi.$$

It also follows from the definitions of $f_\tau(\cdot,t)$ and $Q(\cdot,t)$ in (3.15) that

$$\begin{aligned}\hat{f}_\tau(\cdot,\xi)+\hat{Q}(\cdot,\xi) &= \sum_{n=1}^{\infty}\int_{t_{n-1}}^{t_n}\big(f_\tau(\cdot,t)+Q(\cdot,t)\big)e^{-\xi t}\mathrm{d}t = \sum_{n=1}^{\infty}\int_{t_{n-1}}^{t_n}(f^n+Q^{n-1})e^{-\xi t}\mathrm{d}t\\ &= \frac{e^{\xi\tau}-1}{\xi}\sum_{n=1}^{\infty}(f^n+Q^{n-1})e^{-\xi t_n},\end{aligned}$$

which directly leads to (3.17).

Next, we derive (3.18). Let $\tilde{Z}(\zeta) := \sum_{n=-\infty}^{N}Z^{n-1}\zeta^{N-n} = \sum_{m=0}^{\infty}Z^{N-m-1}\zeta^m$, it has from (3.6) and (3.7) that

$$\sum_{n=-\infty}^{N}({}^{B}\bar{D}_{\tau}^{1-\alpha,x}Z^{n-1})\zeta^{N-n} = \delta_\tau(e^{-\tau\rho V(x)}\zeta)^{1-\alpha}\tilde{Z}(\zeta),$$
$$\sum_{n=-\infty}^{N}({}^{B}\bar{D}_{\tau}^{1,x}Z^{n-1})\zeta^{N-n} = \delta_\tau(e^{-\tau\rho V(x)}\zeta)\tilde{Z}(\zeta).$$

By multiplying ζ^{N-n} on both sides of (3.12) and summing n from $-\infty$ to N, we obtain that

$$\tilde{Z}(\zeta) = \big(\delta_\tau(e^{-\tau\rho V(x)}\zeta)^{\alpha}-\Delta\big)^{-1}\delta_\tau(e^{-\tau\rho V(x)}\zeta)^{\alpha-1}\tilde{M}(\zeta),\ \tilde{M}(\zeta) := \sum_{n=-\infty}^{N}(U^n-u_d^n)\zeta^{N-n},$$

and by Cauchy's integral formula and theorem, it implies

$$Z^{n-1} = \frac{\tau}{2\pi\mathbf{i}}\int_{\Gamma_{\theta,\kappa}^{\tau}} e^{\xi(T-t_n)}\big(\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha}-\Delta\big)^{-1}\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\tilde{M}(e^{-\xi\tau})\mathrm{d}\xi. \tag{3.21}$$

Let $\bar{U}(\cdot,t) = U(\cdot,T-t)$ and $\bar{u}_{d\tau}(\cdot,t) = u_{d\tau}(\cdot,T-t)$, it yields from the definition of $U(\cdot,s)$ and $u_{d\tau}(\cdot,s)$ in (3.16) that the Laplace transform of $\bar{U}(\cdot,t)-\bar{u}_{d\tau}(\cdot,t)$ satisfies

$$\begin{aligned}\hat{\bar{U}}(\cdot,\xi)-\hat{\bar{u}}_{d\tau}(\cdot,\xi) &= \int_0^{\infty}\big(U(\cdot,T-t)-u_{d\tau}(\cdot,T-t)\big)e^{-\xi t}\mathrm{d}t\\ &= \int_{-\infty}^{T}\big(U(\cdot,s)-u_{d\tau}(\cdot,s)\big)e^{-\xi(T-s)}\mathrm{d}s\end{aligned}$$

$$
\begin{aligned}
&= \sum_{n=-\infty}^{N} \int_{t_{n-1}}^{t_n} \big(U(\cdot,s) - u_{d\tau}(\cdot,s)\big) e^{-\xi(T-s)} \mathrm{d}s \\
&= \sum_{n=-\infty}^{N} \int_{t_{n-1}}^{t_n} (U^n - u_d^n) e^{-\xi(T-s)} \mathrm{d}s \\
&= \sum_{n=-\infty}^{N} (U^n - u_d^n) e^{-\xi(T-t_n)} \frac{1-e^{-\xi\tau}}{\xi} \\
&= \tilde{M}(e^{-\xi\tau}) \frac{1-e^{-\xi\tau}}{\xi},
\end{aligned}
$$

which leads to (3.18) by using (3.21). □

To obtain the stability results in Lemma 3.4 for the discrete scheme (3.11)-(3.12), we first introduce a preliminary lemma in the following.

Lemma 3.3 ([6, 29])**.** *Let $\beta(\xi)$ be given by (2.2) and $V(x)$ bounded in $\bar{\Omega}$. By choosing $\theta \in (\frac{\pi}{2}, \pi)$ sufficiently close to $\frac{\pi}{2}$ and $\kappa > 0$ sufficiently large (depending on $|\rho| \|V(x)\|_{L^\infty(\bar{\Omega})}$), there exists a positive constant τ_* such that the following estimates hold for $\tau \le \tau_*$.*

(1) For all $x \in \bar{\Omega}$ and $\xi \in \Sigma_{\theta,\kappa}^{\tau}$, we have $\delta_\tau(e^{-\tau\beta(\xi)}) \in \Sigma_{\frac{3\pi}{4}, C_1\kappa}$ and

$$
C_1|\xi| \le |\delta_\tau(e^{-\tau\beta(\xi)})| \le C_2|\xi|,
$$

where

$$
\Sigma_{\theta,\kappa}^{\tau} = \big\{\xi \in \mathbb{C} : |\xi| \ge \kappa,\ |\arg \xi| \le \theta,\ |\mathrm{Im}(\xi)| \le \frac{\pi}{\tau},\ \mathrm{Re}(\xi) \le \kappa + 1\big\},
$$

$\mathrm{Im}(\xi)$ and $\mathrm{Re}(\xi)$ stand for the imaginary and real parts of ξ, respectively.

(2) The operator $(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta)^{-1} : L^2(\Omega) \to L^2(\Omega)$ is well-defined, bounded, and analytic with respect to $\xi \in \Sigma_{\theta,\kappa}^{\tau}$, satisfying

$$
\begin{aligned}
&\|\Delta(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta)^{-1}\| \le C, \qquad \forall\, \xi \in \Sigma_{\theta,\kappa}^{\tau}, \\
&\|(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta)^{-1}\| \le C|\xi|^{-\alpha}, \quad \forall\, \xi \in \Sigma_{\theta,\kappa}^{\tau}.
\end{aligned}
$$

(3) For all $x \in \bar{\Omega}$ and real number γ, it holds that

$$
|\delta_\tau(e^{-\tau\beta(\xi)})^\gamma - \beta(\xi)^\gamma| \le C\tau|\xi|^{\gamma+1}, \quad \forall\, \xi \in \Gamma_{\theta,\kappa}^{\tau}.
$$

The discrete time-space $\ell^2(L^2(\Omega))$ inner product and norm are introduced as follows for further analysis.

$$
\begin{aligned}
&[\mathbf{v}, \mathbf{w}] = \tau \sum_{n=1}^{N} (v^n, w^n), \quad \forall\, \mathbf{v} = (v^n)_{n=1}^N, \quad \mathbf{w} = (w^n)_{n=1}^N \in L^2(\Omega)^N, \\
&|||\mathbf{v}||| = \sqrt{[\mathbf{v}, \mathbf{v}]} = \Big(\tau \sum_{n=1}^{N} \|v^n\|_{L^2(\Omega)}^2\Big)^{\frac{1}{2}}, \quad \forall\, \mathbf{v} = (v^n)_{n=1}^N \in L^2(\Omega)^N.
\end{aligned}
$$

With above results and the integral representations of the solutions in (3.17)-(3.18), the discrete system (3.11)-(3.12) satisfies the following stability results.

Lemma 3.4. *Let U^n and Z^{n-1} be the solutions to the system (3.11)-(3.12) given by (3.17) and (3.18), respectively. Then we have*

$$
|||\mathbf{U}||| \le C|||\mathbf{f}_\tau + \mathbf{Q}|||, \tag{3.22}
$$

$$
|||\mathbf{Z}||| \le C|||\mathbf{U} - \mathbf{u}_{d\tau}|||, \tag{3.23}
$$

where $\mathbf{f}_\tau = (f^n)_{n=1}^N$ and $\mathbf{u}_{d\tau} = (u_d^n)_{n=1}^N$.

Proof. By Lemma 3.3, we have

$$\begin{aligned}\|E^\tau(t)v\| &\le C\int_{\Gamma^\tau_{\theta,\kappa}} |e^{\xi t}|\cdot\Big|\frac{\xi\tau}{e^{\xi\tau}-1}\Big|\cdot|\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}|\cdot\|(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha-\Delta)^{-1}v\||\mathrm{d}\xi|\\ &\le C\int_{\Gamma^\tau_{\theta,\kappa}} |e^{\xi t}|\cdot|\xi|^{-1}\cdot\|v\||\mathrm{d}\xi|\le C\|v\|, \end{aligned}\tag{3.24}$$

where it utilizes the following estimate [11, Lemma 3.4]:

$$C_0|\xi|\tau\le|1-e^{\xi\tau}|\le C_1|\xi|\tau,\ \ \forall\,\xi\in\Gamma^\tau_{\theta,\kappa}.\tag{3.25}$$

Then it derives from (3.17) that

$$\|U^n\|\le C\int_0^{t_n}\|E^\tau(t_n-s)\|\cdot\|f_\tau(\cdot,s)+Q(\cdot,s)\|\mathrm{d}s\le C\int_0^{t_n}\|f_\tau(\cdot,s)+Q(\cdot,s)\|\mathrm{d}s.$$

With the definition of $f_\tau(\cdot,t)$ and $Q(\cdot,t)$ in (3.15), we obtain (3.22) by

$$\begin{aligned}|||\mathbf{U}|||^2 &\le C\tau\sum_{n=1}^N\Big(\int_0^{t_n}\|f_\tau(\cdot,s)+Q(\cdot,s)\|\mathrm{d}s\Big)^2\\ &\le C\tau\sum_{n=1}^N\sum_{j=1}^n\int_{t_{j-1}}^{t_j}\|f_\tau(\cdot,s)+Q(\cdot,s)\|^2\mathrm{d}s\\ &= C\tau\sum_{n=1}^N\sum_{j=1}^n\int_{t_{j-1}}^{t_j}\|f^j+Q^{j-1}\|^2\mathrm{d}s\\ &\le C|||\mathbf{f}_\tau+\mathbf{Q}|||^2.\end{aligned}$$

By the similar approach, we can derive the estimate (3.23). □

4 Error estimates

In this section, the $\ell^2(L^2(\Omega))$ and $\ell^\infty(L^2(\Omega))$ error estimates of the proposed temporal semi-discrete scheme (3.4)-(3.5) are rigorously established without the regularity requirement on the solutions of the optimality system. The main results are stated in the following theorems.

Theorem 4.1 ($\ell^2(L^2(\Omega))$ error)**.** *Let (u,z,q) and (U^n,Z^{n-1},Q^{n-1}) be the solutions of the problems (2.10)-(2.12) and (3.11)-(3.13), respectively. If $f,u_d\in L^2(0,T;L^2(\Omega))$, $V(x)\in W^{2,\infty}(\Omega)$ and $\mathrm{Re}(\rho V(x))\ge 0$, then we have*

$$|||\mathbf{u}-\mathbf{U}|||+|||\mathbf{z}-\mathbf{Z}|||+|||\mathbf{q}-\mathbf{Q}|||\le Cl_\tau\tau,$$

where $\mathbf{u}=(u(\cdot,t_n))_{n=1}^N$, $\mathbf{z}=(z(\cdot,t_{n-1}))_{n=1}^N$, $\mathbf{q}=(q(\cdot,t_{n-1}))_{n=1}^N$, $l_\tau=\ln(\frac{1}{\tau})$, and the constant C is independent of n,τ.

Theorem 4.2 ($\ell^\infty(L^2(\Omega))$ error)**.** *Let (u,z,q) and (U^n,Z^{n-1},Q^{n-1}) be the solutions of the problems (2.10)-(2.12) and (3.11)-(3.13), respectively. If $f,u_d\in H^1(0,T;L^2(\Omega))$, $V(x)\in W^{2,\infty}(\Omega)$ and $\mathrm{Re}(\rho V(x))\ge 0$, then we have*

$$\max_{1\le n\le N}\left\{\|u(t_n)-U^n\|+\|z(t_{n-1})-Z^{n-1}\|+\|q(t_{n-1})-Q^{n-1}\|\right\}\le Cl_\tau\tau,$$

where $l_\tau=\ln(\frac{1}{\tau})$, and the constant C is independent of n,τ.

4.1 Some lemmas

To prove the error estimate in Theorem 4.1, we first derive some lemmas in this subsection.

Lemma 4.3. *Let $E(\cdot)$ and $E^\tau(\cdot)$ be given by* (2.20) *and* (3.19)*, respectively, and*

$$K^n := \int_0^{t_n} \big(E(t_n - s) - E^\tau(t_n - s)\big)\big(f(\cdot, s) + q(\cdot, s)\big)\mathrm{d}s.$$

Then we have

$$|||(K^n)_{n=1}^N||| \le C l_\tau \tau,$$

where $l_\tau = \ln(\frac{1}{\tau})$ and the constant C is independent of n, τ.

Proof. From (2.20) and (3.19), we obtain

$$K^n = \int_0^{t_n} \big(B_1(t_n - s) + B_2(t_n - s)\big)\big(f(\cdot, s) + q(\cdot, s)\big)\mathrm{d}s,$$

where

$$B_1(t) = \frac{1}{2\pi \mathbf{i}} \int_{\Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau} e^{\xi t}\hat{B}_1(\xi)\mathrm{d}\xi, \quad B_2(t) = \frac{1}{2\pi \mathbf{i}} \int_{\Gamma_{\theta,\kappa}^\tau} e^{\xi t}\hat{B}_2(\xi)\mathrm{d}\xi, \tag{4.1}$$

with

$$\begin{aligned}
\hat{B}_1(\xi) &= \beta(\xi)^{\alpha-1}\big(\beta(\xi)^\alpha - \Delta\big)^{-1}, \\
\hat{B}_2(\xi) &= \beta(\xi)^{\alpha-1}\big(\beta(\xi)^\alpha - \Delta\big)^{-1} - \frac{\xi\tau}{e^{\xi\tau} - 1}\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}.
\end{aligned}$$

By (3.25), Lemmas 2.2 and 3.3, it holds that

$$\|\hat{B}_1(\xi)\| \le C|\xi|^{-1}, \ \ \forall\, \xi \in \Gamma_{\theta,\kappa}, \ \text{ and } \ \|\hat{B}_2(\xi)\| \le C|\xi|^{-1}, \ \ \forall\, \xi \in \Gamma_{\theta,\kappa}^\tau. \tag{4.2}$$

In addition, we have $\|\hat{B}_1(\xi)\| \le C\tau$ for any $\xi \in \Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau$, and

$$\begin{aligned}
\|\hat{B}_2(\xi)\| &= \big\|\big(\beta(\xi)^{\alpha-1} - \delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\big)\big(\beta(\xi)^\alpha - \Delta\big)^{-1}\big\| \\
&\quad + \big\|\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\big[\big(\beta(\xi)^\alpha - \Delta\big)^{-1} - \big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\big]\big\| \\
&\quad + \Big\|\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}\Big[\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\Big(1 - \frac{\xi\tau}{e^{\xi\tau} - 1}\Big)\Big]\Big\| \\
&\le C\tau|\xi|^\alpha|\xi|^{-\alpha} + C|\xi|^{\alpha-1}|\xi|^{-\alpha}\tau|\xi|^{\alpha+1}|\xi|^{-\alpha} + C|\xi|^{\alpha-1}|\xi|^{-\alpha}|\xi|\tau \\
&= C\tau, \ \ \forall\, \xi \in \Gamma_{\theta,\kappa}^\tau,
\end{aligned} \tag{4.3}$$

where it applies Lemma 3.3 and the following estimate

$$\left|1 - \frac{\xi\tau}{e^{\xi\tau} - 1}\right| = |\delta_\tau(e^{-\xi\tau})^{-1}(\delta_\tau(e^{-\xi\tau}) - \xi)| \le C|\xi|\tau, \ \ \forall\, \xi \in \Gamma_{\theta,\kappa}^\tau,$$

which is obtained by using [11, Lemma 3.4]. Combining (4.2) and (4.3), we obtain

$$\|\hat{B}_1(\xi)\| \le C\tau^{1-\epsilon}|\xi|^{-\epsilon}, \ \ \forall\, \xi \in \Gamma_{\theta,\kappa}\backslash\Gamma_{\theta,\kappa}^\tau, \ \epsilon \in (0,1), \tag{4.4}$$

$$\|\hat{B}_2(\xi)\| \le C\tau^{1-\epsilon}|\xi|^{-\epsilon}, \ \ \forall\, \xi \in \Gamma_{\theta,\kappa}^\tau, \ \epsilon \in (0,1). \tag{4.5}$$

Then we derive from (4.1) that

$$\begin{aligned}
\|B_1(t)\| &\le C\tau^{1-\epsilon}t^{-(1-\epsilon)}, \ \ \forall\, \epsilon \in (0,1), \ t \in (0,T], \\
\|B_2(t)\| &\le C\tau^{1-\epsilon}t^{-(1-\epsilon)}, \ \ \forall\, \epsilon \in (0,1), \ t \in (0,T].
\end{aligned}$$

Moreover, it obtains from (2.23) and (3.24) that

$$\begin{aligned}\|K^n\| \leq & \int_0^{t_{n-1}} \|B_1(t_n-s)+B_2(t_n-s)\| \cdot \|f(\cdot,s)+q(\cdot,s)\| \mathrm{d}s \\ & + \int_{t_{n-1}}^{t_n} \|E(t_n-s)-E^\tau(t_n-s)\| \cdot \|f(\cdot,s)+q(\cdot,s)\| \mathrm{d}s \\ \leq & C\tau^{1-\epsilon} \int_0^{t_{n-1}} \frac{(t_n+\tau-s)^{1-\epsilon}}{(t_{n-1}+\tau-s)^{1-\epsilon}} (t_n+\tau-s)^{-(1-\epsilon)} \|f(\cdot,s)+q(\cdot,s)\| \mathrm{d}s \\ & + \tau^{1-\epsilon} \int_{t_{n-1}}^{t_n} (t_n+\tau-s)^{-(1-\epsilon)} \|f(\cdot,s)+q(\cdot,s)\| \mathrm{d}s \\ \leq & C\tau^{1-\epsilon} \int_0^T \mathbf{1}_{\{t_n>s\}} (t_n+\tau-s)^{-(1-\epsilon)} \|f(\cdot,s)+q(\cdot,s)\| \mathrm{d}s, \quad \epsilon \in (0,1).\end{aligned} \tag{4.6}$$

Then, by using the following two inequalities [12]

$$\max_{1\leq n\leq N} \int_0^T \mathbf{1}_{t_n>s} (t_n+\tau-s)^{-(1-\epsilon)} \mathrm{d}s \leq C\epsilon^{-1}(t_n+\tau)^\epsilon \leq C\epsilon^{-1}, \tag{4.7}$$

$$\sup_{s\in(0,T)} \tau \sum_{n=1}^N \mathbf{1}_{t_n>s} (t_n+\tau-s)^{-(1-\epsilon)} \leq \sup_{s\in(0,T)} \int_{s-\tau}^T (t+\tau-s)^{-(1-\epsilon)} \mathrm{d}t \leq C\epsilon^{-1}, \tag{4.8}$$

we can derive that

$$\begin{aligned}& |||(K^n)_{n=1}^N||| = \Big(\tau \sum_{n=1}^N \|K^n\|^2\Big)^{\frac{1}{2}} \\ & \leq C\Big(\tau \sum_{n=1}^N \tau^{2-2\epsilon} \Big[\int_0^T \mathbf{1}_{\{t_n>s\}} (t_n+\tau-s)^{-(1-\epsilon)} \|f(\cdot,s)+q(\cdot,s)\| \mathrm{d}s\Big]^2\Big)^{\frac{1}{2}} \\ & \leq C\tau^{1-\epsilon} \Big(\tau \sum_{n=1}^N \int_0^T \mathbf{1}_{\{t_n>s\}} (t_n+\tau-s)^{-(1-\epsilon)} \mathrm{d}s \\ & \qquad \cdot \int_0^T \mathbf{1}_{\{t_n>s\}} (t_n+\tau-s)^{-(1-\epsilon)} \|f(\cdot,s)+q(\cdot,s)\|^2 \mathrm{d}s\Big)^{\frac{1}{2}} \\ & \leq C\tau^{1-\epsilon} \Big(\epsilon^{-1} \tau \sum_{n=1}^N \int_0^T \mathbf{1}_{\{t_n>s\}} (t_n+\tau-s)^{-(1-\epsilon)} \|f(\cdot,s)+q(\cdot,s)\|^2 \mathrm{d}s\Big)^{\frac{1}{2}} \\ & \leq C\tau^{1-\epsilon} \Big(\epsilon^{-2} \int_0^T \|f(\cdot,s)+q(\cdot,s)\|^2 \mathrm{d}s\Big)^{\frac{1}{2}} \\ & \leq C\tau^{1-\epsilon}\epsilon^{-1} \|f+q\|_{L^2(0,T;L^2(\Omega))} \\ & \leq C\tau^{1-\epsilon}\epsilon^{-1} = Cl_\tau \tau,\end{aligned}$$

where $\epsilon = l_\tau^{-1}$ is taken with $l_\tau = \ln(1/\tau)$. □

Lemma 4.4. *Let $E^\tau(\cdot)$ and $f_\tau(\cdot,t)$ be defined by (3.19) and (3.15), respectively,*

$$L^n := \int_0^{t_n} E^\tau(t_n-s)\big(f(\cdot,s)-f_\tau(\cdot,s)\big) \mathrm{d}s.$$

Then we have

$$|||(L^n)_{n=1}^N||| \leq Cl_\tau \tau,$$

where $l_\tau = \ln(1/\tau)$ and the constant C is independent of n, τ.

Proof. We have from (3.15) and $f^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} f(\cdot,t)\mathrm{d}t$ in (3.5) that

$$\begin{aligned}\int_{t_{j-1}}^{t_j} E^\tau(t_n - t_{j-1}) f_\tau(\cdot,s)\mathrm{d}s &= \int_{t_{j-1}}^{t_j} E^\tau(t_n - t_{j-1})\frac{1}{\tau}\int_{t_{j-1}}^{t_j} f(\cdot,w)\mathrm{d}w\mathrm{d}s \\ &= \int_{t_{j-1}}^{t_j} E^\tau(t_n - t_{j-1}) f(\cdot,s)\mathrm{d}s.\end{aligned}$$

Then it follows from (3.24) that

$$\begin{aligned}\|L^n\| &= \Big\| \sum_{j=1}^n \int_{t_{j-1}}^{t_j} E^\tau(t_n - s)\big(f(\cdot,s) - f_\tau(\cdot,s)\big)\mathrm{d}s \Big\| \\ &= \Big\| \sum_{j=1}^n \int_{t_{j-1}}^{t_j} \big(E^\tau(t_n - s) - E^\tau(t_n - t_{j-1})\big)\big(f(\cdot,s) - f_\tau(\cdot,s)\big)\mathrm{d}s \Big\| \\ &\le \sum_{j=1}^n \int_{t_{j-1}}^{t_j} \|E^\tau(t_n - s) - E^\tau(t_n - t_{j-1})\| \cdot \|f(\cdot,s) - f_\tau(\cdot,s)\|\mathrm{d}s \\ &\le \sum_{j=1}^{n-1} \int_{t_{j-1}}^{t_j} C\tau^{1-\epsilon}(t_n - s)^{-(1-\epsilon)}\|f(\cdot,s) - f_\tau(\cdot,s)\|\mathrm{d}s \\ &\quad + \int_{t_{n-1}}^{t_n} \big(\|E^\tau(t_n - s)\| + \|E^\tau(t_n - t_{j-1})\|\big)\|f(\cdot,s) - f_\tau(\cdot,s)\|\mathrm{d}s \\ &\le C\tau^{1-\epsilon}\int_0^{t_{n-1}} (t_n - s)^{-(1-\epsilon)}\|f(\cdot,s) - f_\tau(\cdot,s)\|\mathrm{d}s + \int_{t_{n-1}}^{t_n} \|f(\cdot,s) - f_\tau(\cdot,s)\|\mathrm{d}s,\end{aligned}$$

where we use the following estimate

$$\begin{aligned}&\|E^\tau(t_n - s) - E^\tau(t_n - t_{j-1})\| \\ &\le C\int_{\Gamma^\tau_{\theta,\kappa}} \big|e^{\xi(t_n - s)} - e^{\xi(t_n - t_{j-1})}\big| \cdot \Big|\frac{\xi\tau}{e^{\xi\tau} - 1}\Big| \\ &\qquad \cdot |\delta_\tau(e^{-\tau\beta(\xi)})^{\alpha-1}| \cdot \big\|\big(\delta_\tau(e^{-\tau\beta(\xi)})^\alpha - \Delta\big)^{-1}\big\| \cdot |\mathrm{d}\xi| \\ &\le C\int_{\Gamma^\tau_{\theta,\kappa}} |e^{\xi(t_n - s)}| \cdot |1 - e^{\xi(s - t_{j-1})}| \cdot |\xi|^{-1} \cdot |\mathrm{d}\xi| \\ &\le C\int_{\Gamma^\tau_{\theta,\kappa}} |e^{\xi(t_n - s)}| \cdot \tau^{1-\epsilon}|\xi|^{-\epsilon} \cdot |\mathrm{d}\xi| \\ &\le C\tau^{1-\epsilon}(t_n - s)^{-(1-\epsilon)}, \quad s \in (t_{j-1}, t_j).\end{aligned}$$

Similar to the estimate of K^n in Lemma 4.3, we have

$$\|L^n\| \le C\tau^{1-\epsilon}\int_0^T \mathbf{1}_{\{t_n > s\}}(t_n + \tau - s)^{-(1-\epsilon)}\|f(\cdot,s) - f_\tau(\cdot,s)\|\mathrm{d}s, \ \epsilon \in (0,1),$$

which further yields

$$\|\|(L^n)_{n=1}^N\|\| \le C\tau^{1-\epsilon}\epsilon^{-1}\|f - f_\tau\|_{L^2(0,T;L^2(\Omega))} \le C\tau^{1-\epsilon}\epsilon^{-1} \le Cl_\tau\tau.$$

The proof is completed. ◻

Lemma 4.5. *Let $E^\tau(\cdot)$ be defined by (3.19) and*

$$J^n := \int_0^{t_n} E^\tau(t_n - s)\big(q(\cdot,s) - q_\tau(\cdot,s)\big)\mathrm{d}s,$$

where $q_\tau(\cdot,t)|_{[t_{n-1},t_n)} = q(\cdot,t_{n-1})$ *for* $n=1,2,\cdots,N$. *Then we have*

$$|||(J^n)_{n=1}^N||| \le C\tau,$$

where C *is a constant independent of* n,τ.

Proof. It obtains from (3.24) that

$$\begin{aligned}
\|J^n\| &\le \int_0^{t_n} \|E^\tau(t_n-s)\|\cdot\|q(\cdot,s)-q_\tau(\cdot,s)\|\mathrm{d}s \\
&\le C\int_0^{t_n} \|q(\cdot,s)-q_\tau(\cdot,s)\|\mathrm{d}s \\
&= C\sum_{j=1}^n \int_{t_{j-1}}^{t_j} \|q(\cdot,s)-q(\cdot,t_{j-1})\|\mathrm{d}s \\
&\le C\sum_{j=1}^n \int_{t_{j-1}}^{t_j}\int_{t_{j-1}}^{s} \|\partial_\xi q(\cdot,\xi)\|\mathrm{d}\xi\mathrm{d}s \\
&\le C\tau\int_0^{t_n} \|\partial_s q(\cdot,s)\|\mathrm{d}s.
\end{aligned} \tag{4.9}$$

Recalling the prior regularity estimate of q obtained in Theorem 2.7, then we have

$$\begin{aligned}
|||(J^n)_{n=1}^N|||^2 &\le C\tau\sum_{n=1}^N \tau^2\Big(\int_0^{t_n} \|\partial_s q(\cdot,s)\|\mathrm{d}s\Big)^2 \\
&\le C\tau^2\int_0^T \|\partial_s q(\cdot,s)\|^2\mathrm{d}s \\
&\le C\tau^2\|q\|^2_{H^1(0,T;L^2(\Omega))} \\
&\le C\tau^2,
\end{aligned}$$

which completes the proof. □

With the estimates in Lemmas 4.3, 4.4 and 4.5, we can derive the following lemma.

Lemma 4.6. *Let* u *be the solution to the state equation* (2.10)*, and* $\mathbf{U}(\mathbf{q}) := (U(q)^n)_{n=1}^N$ *with* $U(q)^n$ *being the solution to the following semi-discrete equation*

$$\begin{cases} \bar{D}_\tau^{1,x}U(q)^n - \Delta\bar{D}_\tau^{1-\alpha,x}U(q)^n = f^n + q^{n-1}, & x\in\Omega, \quad n=1,2,\cdots,N, \\ U(q)^0 = 0, \quad x\in\Omega, \quad \text{and} \quad U(q)^n = 0, & x\in\partial\Omega, \quad n=0,1,\cdots,N, \end{cases} \tag{4.10}$$

where $f^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} f(\cdot,t)\mathrm{d}t$ *and* $q^{n-1} = q(\cdot,t_{n-1})$. *Then we have*

$$|||\mathbf{u}-\mathbf{U}(\mathbf{q})||| \le Cl_\tau\tau. \tag{4.11}$$

Proof. We have from the solution representations in (2.18) and (3.17) that

$$\begin{aligned}
u(\cdot,t_n) - U(q)^n &= \int_0^{t_n} E(t_n-s)\big(f(\cdot,s)+q(\cdot,s)\big)\mathrm{d}s \\
&\quad - \int_0^{t_n} E^\tau(t_n-s)\big(f_\tau(\cdot,s)+q_\tau(\cdot,s)\big)\mathrm{d}s \\
&:= K^n + L^n + J^n,
\end{aligned} \tag{4.12}$$

where K^n, L^n and J^n are given in Lemmas 4.3, 4.4 and 4.5, respectively, and

$$f_\tau(\cdot,t)|_{(t_{n-1},t_n]} = f^n, \;\; q_\tau(\cdot,t)|_{[t_{n-1},t_n)} = q^{n-1} = q(\cdot,t_{n-1}),$$

for $n=1,2,\cdots,N$. By Lemmas 4.3, 4.4 and 4.5, we obtain the result (4.11). □

By the similar approach as above, the following estimate can also be derived.

Lemma 4.7. *Let z be the solution to the adjoint equation (2.11), and $\mathbf{Z}(\mathbf{u}) := (Z(u)^{n-1})_{n=1}^{N}$ with $Z(u)^{n-1}$ being the solution to the following equation*

$$\begin{cases} {}^B\bar{D}_\tau^{1,x} Z(u)^{n-1} - {}^B\bar{D}_\tau^{1-\alpha,x}\Delta Z(u)^{n-1} = u^n - u_d^n, \;\; x\in\Omega, \;\; n = N,\cdots,1, \\ Z(u)^N = 0, \;\; x\in\Omega, \; \textit{and } Z(u)^n = 0, \; x\in\partial\Omega, \;\; n = N,\cdots,1,0, \end{cases} \tag{4.13}$$

where $u^n = u(\cdot,t_n)$ and $u_d^n = \frac{1}{\tau}\int_{t_{n-1}}^{t_n} u_d(\cdot,t)\mathrm{d}t$. Then we have

$$|||\mathbf{z} - \mathbf{Z}(\mathbf{u})||| \le C l_\tau \tau. \tag{4.14}$$

Proof. By (2.19) and (3.18), we have

$$\begin{aligned} z(\cdot,t_{n-1}) - Z(u)^{n-1} &= \int_{t_{n-1}}^{T} F(s-t_{n-1})\big(u(\cdot,s) - u_d(\cdot,s)\big)\mathrm{d}s \\ &\quad - \int_{t_{n-1}}^{T} F^\tau(s-t_{n-1})\big(u_\tau(\cdot,s) - u_{d\tau}(\cdot,s)\big)\mathrm{d}s \\ &= \int_{t_{n-1}}^{T} \big(F(s-t_{n-1}) - F^\tau(s-t_{n-1})\big)\big(u(\cdot,s) - u_d(\cdot,s)\big)\mathrm{d}s \\ &\quad + \int_{t_{n-1}}^{T} F^\tau(s-t_{n-1})\big(u(\cdot,s) - u_\tau(\cdot,s)\big)\mathrm{d}s \\ &\quad - \int_{t_{n-1}}^{T} F^\tau(s-t_{n-1})\big(u_d(\cdot,s) - u_{d\tau}(\cdot,s)\big)\mathrm{d}s, \end{aligned}$$

where $u_\tau(\cdot,t)|_{(t_{n-1},t_n]} = u^n = u(\cdot,t_n)$ and $u_{d\tau}(\cdot,t)|_{(t_{n-1},t_n]} = u_d^n$ for $n = 1,2,\cdots,N$. Analogous to the proofs of Lemmas 4.3, 4.4 and 4.5, we can obtain the result (4.14). □

4.2 Proof of Theorem 4.1

Based on the lemmas in the above subsection, we can demonstrate the proof of Theorem 4.1.

Proof of Theorem 4.1. As $q(\cdot,t_{n-1}) = P_{U_{ad}}(-\frac{1}{\gamma}z(\cdot,t_{n-1}))$ due to (2.15), we have

$$\big(\gamma q(\cdot,t_{n-1}) + z(\cdot,t_{n-1}), v - q(\cdot,t_{n-1})\big) \ge 0, \;\; \forall\, v\in L^2(\Omega), \; a\le v\le b.$$

Then it follows from the above variational inequality and (3.13) that

$$\begin{aligned} [\gamma\mathbf{q}, \mathbf{q}-\mathbf{Q}] &= -[\mathbf{z}, \mathbf{q}-\mathbf{Q}] - [\gamma\mathbf{q}+\mathbf{z}, \mathbf{Q}-\mathbf{q}] \le -[\mathbf{z}, \mathbf{q}-\mathbf{Q}], \\ -[\gamma\mathbf{Q}, \mathbf{q}-\mathbf{Q}] &= [\mathbf{Z}, \mathbf{q}-\mathbf{Q}] - [\gamma\mathbf{Q}+\mathbf{Z}, \mathbf{q}-\mathbf{Q}] \le [\mathbf{Z}, \mathbf{q}-\mathbf{Q}], \end{aligned}$$

which further leads to

$$\begin{aligned} \gamma|||\mathbf{q}-\mathbf{Q}|||^2 &= \gamma[\mathbf{q}, \mathbf{q}-\mathbf{Q}] - \gamma[\mathbf{Q}, \mathbf{q}-\mathbf{Q}] \\ &\le -[\mathbf{z}, \mathbf{q}-\mathbf{Q}] + [\mathbf{Z}, \mathbf{q}-\mathbf{Q}] \\ &= [\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q})), \mathbf{q}-\mathbf{Q}] + [\mathbf{Z}(\mathbf{U}(\mathbf{q})) - \mathbf{z}, \mathbf{q}-\mathbf{Q}], \end{aligned}$$

where $\mathbf{U}(\mathbf{q}) = (U(q)^n)_{n=1}^N$ with $U(q)^n$ being the solution to (4.10), and $\mathbf{Z}(\mathbf{U}(\mathbf{q})) = (Z(U(q))^n)_{n=1}^N$ with $Z(U(q))^n$ being the solution to (4.13) replacing u^n by $U(q)^n$. Then by (3.8) and (3.9), we deduce

$$\begin{aligned} [\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q})), \mathbf{q}-\mathbf{Q}] &= [\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q})), (\bar{D}_\tau^{1,x} - \Delta\bar{D}_\tau^{1-\alpha,x})(\mathbf{U}(\mathbf{q})-\mathbf{U})] \\ &= [({}^B\bar{D}_\tau^{1,x} - {}^B\bar{D}_\tau^{1-\alpha,x}\Delta)(\mathbf{Z}-\mathbf{Z}(\mathbf{U}(\mathbf{q}))), \mathbf{U}(\mathbf{q})-\mathbf{U}] \end{aligned}$$

$$= -|||\mathbf{U}(\mathbf{q}) - \mathbf{U}|||^2 \leq 0,$$

which implies that

$$\begin{aligned} |||\mathbf{q} - \mathbf{Q}||| &\leq C|||\mathbf{Z}(\mathbf{U}(\mathbf{q})) - \mathbf{z}||| \\ &\leq C|||\mathbf{Z}(\mathbf{U}(\mathbf{q})) - \mathbf{Z}(\mathbf{u})||| + C|||\mathbf{Z}(\mathbf{u}) - \mathbf{z}||| \\ &\leq C|||\mathbf{U}(\mathbf{q}) - \mathbf{u}||| + C|||\mathbf{Z}(\mathbf{u}) - \mathbf{z}||| \\ &\leq Cl_\tau \tau, \end{aligned} \tag{4.15}$$

where the estimates in Lemmas 3.4, 4.6 and 4.7 are applied.

It follows from Lemma 3.4 that

$$|||\mathbf{U}(\mathbf{q}) - \mathbf{U}||| \leq C|||\mathbf{q} - \mathbf{Q}|||.$$

Then the result in Lemma 4.6 leads to

$$|||\mathbf{u} - \mathbf{U}||| \leq |||\mathbf{u} - \mathbf{U}(\mathbf{q})||| + |||\mathbf{U}(\mathbf{q}) - \mathbf{U}||| \leq |||\mathbf{u} - \mathbf{U}(\mathbf{q})||| + C|||\mathbf{q} - \mathbf{Q}||| \leq Cl_\tau \tau.$$

By using the triangle inequality, Lemmas 3.4 and 4.7, we obtain

$$\begin{aligned} |||\mathbf{z} - \mathbf{Z}||| &\leq |||\mathbf{z} - \mathbf{Z}(\mathbf{u})||| + |||\mathbf{Z}(\mathbf{u}) - \mathbf{Z}||| \\ &\leq |||\mathbf{z} - \mathbf{Z}(\mathbf{u})||| + C|||\mathbf{u} - \mathbf{U}||| \\ &\leq Cl_\tau \tau. \end{aligned} \tag{4.16}$$

The proof is completed. □

4.3 Proof of Theorem 4.2

Proof of Theorem 4.2. We first estimate $\max_{1\leq n\leq N} \|u(t_n) - U^n\|$ by splitting $u(t_n) - U^n$ into two parts: $u(t_n) - U(q)^n$ and $U(q)^n - U^n$, where $U(q)^n$ is the solution to (4.10).

For $u(t_n) - U^n$, we need to analyze each term in (4.12). By using (4.6), (4.7) and the Sobolev imbedding $H^1(0,T) \hookrightarrow L^\infty(0,T)$, we can obtain

$$\begin{aligned} \max_{1\leq n\leq N} \|K^n\| &\leq C\tau^{1-\epsilon} \max_{1\leq n\leq N} \int_0^T \mathbf{1}_{\{t_n>s\}} (t_n + \tau - s)^{-(1-\epsilon)} \|f(\cdot,s) + q(\cdot,s)\| \mathrm{d}s \\ &\leq C\tau^{1-\epsilon}\epsilon^{-1} \|f + q\|_{L^\infty(0,T;L^2(\Omega))} \\ &\leq Cl_\tau \tau \|f + q\|_{H^1(0,T;L^2(\Omega))}, \end{aligned}$$

where $q \in H^1(0,T;L^2(\Omega)$ has been proved in Theorem 2.7. From the definition of L^n in Lemma 4.4 and the estimate (3.24), it follows that

$$\begin{aligned} \max_{1\leq n\leq N} \|L^n\| &\leq \max_{1\leq n\leq N} \int_0^{t_n} \|E^\tau(t_n - s)\| \cdot \|f(\cdot,s) - f_\tau(\cdot,s)\| \mathrm{d}s \\ &\leq C \int_0^T \left\|f(\cdot,s) - f_\tau(\cdot,s)\right\| \mathrm{d}s \\ &= C \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \left\| f(\cdot,s) - \frac{1}{\tau} \int_{t_{j-1}}^{t_j} f(\cdot,r) \mathrm{d}r \right\| \mathrm{d}s \\ &\leq C \sum_{j=1}^N \int_{t_{j-1}}^{t_j} \int_{t_{j-1}}^{t_j} \|\partial_\xi f(\cdot,\xi)\| \mathrm{d}\xi \mathrm{d}s \\ &\leq C\tau \|f\|_{H^1(0,T;L^2(\Omega))}. \end{aligned}$$

In addition, the estimate (4.9) directly leads to

$$\max_{1\leq n\leq N} \|J^n\| \leq C\tau \|q\|_{H^1(0,T;L^2(\Omega))}.$$

Then the above estimates and (4.12) imply that

$$\max_{1\le n\le N}\|u(t_n)-U(q)^n\|\le Cl_\tau\tau. \tag{4.17}$$

It obtains from the solution representation (3.17), the estimates (3.24) and (4.15) that

$$\begin{aligned}\max_{1\le n\le N}\|U(q)^n-U^n\| &\le \max_{1\le n\le N}\int_0^{t_n}\|E^\tau(t_n-s)\|\cdot\|q_\tau(\cdot,s)-Q(\cdot,s)\|\mathrm{d}s\\ &\le C\int_0^T\|q_\tau(\cdot,s)-Q(\cdot,s)\|\mathrm{d}s\\ &= C\tau\sum_{j=1}^N\left\|q(\cdot,t_{j-1})-Q^{j-1}\right\|\\ &\le C|||\mathbf{q}-\mathbf{Q}|||\le Cl_\tau\tau.\end{aligned} \tag{4.18}$$

Thus, the estimates (4.17) and (4.18) imply that

$$\begin{aligned}\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))} :&= \max_{1\le n\le N}\|u(t_n)-U^n\|\\ &\le \max_{1\le n\le N}\left\{\|u(t_n)-U(q)^n\|+\|U(q)^n-U^n\|\right\}\\ &\le Cl_\tau\tau.\end{aligned}$$

By the similar approach as above, we can also derive

$$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}:=\max_{1\le n\le N}\|z(t_{n-1})-Z^{n-1}\|\le Cl_\tau\tau.$$

With the contraction property of the projection $P_{U_{ad}}(\cdot)$ (see [16, Corollary 2.4]) given by (2.16), we obtain from (2.15) and (3.14) that

$$\begin{aligned}\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))} :&= \max_{1\le n\le N}\|q(t_{n-1})-Q^{n-1}\|\\ &= \max_{1\le n\le N}\left\|P_{U_{ad}}\big(-\frac{1}{\gamma}z(t_{n-1})\big)-P_{U_{ad}}\big(-\frac{1}{\gamma}Q^{n-1}\big)\right\|\\ &\le C\max_{1\le n\le N}\|z(t_{n-1})-Z^{n-1}\|\\ &\le Cl_\tau\tau.\end{aligned}$$

The proof is completed. □

5 Numerical results

In this section, we verify the theoretical error estimates of the proposed temporal discrete scheme for the optimal control problem governed by the forward fractional Feynman-Kac equation through numerical experiments. We solve the discrete optimal control problem (3.4)-(3.5) by the inexact alternating direction method of multipliers (ADMM) algorithm [8] with the piecewise linear finite element discretization in space, where the Lagrange penalty parameter is taken as 1 and the tolerance is 1.0×10^{-5}.

Example 5.1. *We consider the problem* (1.4)-(1.5) *in one-dimensional case. Let* $\Omega=(0,1),\ T=1,\ \gamma=1,\ V(x)=x$ *and* $\rho=1$. *The exact solutions are chosen as*

$$\begin{aligned}u(x,t)&=e^{-t\rho x}tx(1-x),\\ z(x,t)&=e^{t\rho x}(1-t)x(1-x),\\ q(x,t)&=\max\{-0.1,\min\{-z(x,t),-0.01\}\},\end{aligned}$$

with f *and* u_d *being calculated by* (2.10) *and* (2.11) *correspondingly to the exact solutions.*

We let $\alpha = 0.2, 0.5, 0.8$ and choose $\tau = 1/8, 1/16, 1/32, 1/64$ to solve the problem (3.4)-(3.5) with the finite element mesh of equal subintervals in $\Omega = (0,1)$ and the mesh size $h = 1/64$. In Table 1, the $\ell^2(L^2(\Omega))$ errors $|||\mathbf{u}-\mathbf{U}|||$, $|||\mathbf{z}-\mathbf{Z}|||$, $|||\mathbf{q}-\mathbf{Q}|||$ and the numerical convergence orders in time direction are presented for Example 5.1, which is consistent with the theoretical order of $O(\tau)$ in Theorem 4.1. In addition, it can be observed that our numerical scheme is effective, and the convergence order is not affected by the fractional order α. Table 2 provides the $\ell^\infty(L^2(\Omega))$ errors and the corresponding numerical convergence orders for Example 5.1, which also confirms the theoretical estimate in Theorem 4.2.

Table 1: The $\ell^2(L^2(\Omega))$ errors and numerical convergence orders for Example 5.1.

α	$\ell^2(L^2(\Omega))$ error	$\tau = 1/8$	$\tau = 1/16$	$\tau = 1/32$	$\tau = 1/64$	Order
0.2	$\|\|\|\mathbf{u}-\mathbf{U}\|\|\|$	1.67e-03	8.26e-04	4.02e-04	1.95e-04	$\approx$ 1.03 (1.0)
	$\|\|\|\mathbf{z}-\mathbf{Z}\|\|\|$	2.64e-03	1.33e-03	6.65e-04	3.31e-04	$\approx$ 1.00 (1.0)
	$\|\|\|\mathbf{q}-\mathbf{Q}\|\|\|$	2.02e-03	1.01e-03	4.73e-04	2.14e-04	$\approx$ 1.08 (1.0)
0.5	$\|\|\|\mathbf{u}-\mathbf{U}\|\|\|$	2.73e-03	1.36e-03	6.75e-04	3.34e-04	$\approx$ 1.01 (1.0)
	$\|\|\|\mathbf{z}-\mathbf{Z}\|\|\|$	3.85e-03	1.93e-03	9.61e-04	4.76e-04	$\approx$ 1.00 (1.0)
	$\|\|\|\mathbf{q}-\mathbf{Q}\|\|\|$	3.31e-03	1.67e-03	8.19e-04	4.03e-04	$\approx$ 1.01 (1.0)
0.8	$\|\|\|\mathbf{u}-\mathbf{U}\|\|\|$	4.69e-03	2.37e-03	1.19e-03	5.96e-04	$\approx$ 0.99 (1.0)
	$\|\|\|\mathbf{z}-\mathbf{Z}\|\|\|$	7.04e-03	3.57e-03	1.80e-03	9.04e-04	$\approx$ 0.99 (1.0)
	$\|\|\|\mathbf{q}-\mathbf{Q}\|\|\|$	5.04e-03	2.58e-03	1.31e-03	6.61e-04	$\approx$ 0.98 (1.0)

Table 2: The $\ell^\infty(L^2(\Omega))$ errors and numerical convergence orders for Example 5.1.

α	$\ell^\infty(L^2(\Omega))$ error	$\tau = 1/8$	$\tau = 1/16$	$\tau = 1/32$	$\tau = 1/64$	Order
0.2	$\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))}$	3.02e-03	1.63e-03	8.40e-04	4.20e-04	$\approx$ 0.95 (1.0)
	$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}$	4.83e-03	2.71e-03	1.42e-03	7.16e-04	$\approx$ 0.92 (1.0)
	$\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))}$	4.82e-03	2.67e-03	1.21e-03	5.89e-04	$\approx$ 1.01 (1.0)
0.5	$\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))}$	4.25e-03	2.09e-03	1.04e-03	5.16e-04	$\approx$ 1.01 (1.0)
	$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}$	7.00e-03	3.53e-03	1.74e-03	8.64e-04	$\approx$ 1.01 (1.0)
	$\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))}$	6.98e-03	3.46e-03	1.72e-03	8.53e-04	$\approx$ 1.01 (1.0)
0.8	$\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))}$	5.85e-03	3.01e-03	1.53e-03	7.72e-04	$\approx$ 0.97 (1.0)
	$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}$	9.49e-03	4.94e-03	2.51e-03	1.27e-03	$\approx$ 0.97 (1.0)
	$\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))}$	9.48e-03	4.93e-03	2.51e-03	1.27e-03	$\approx$ 0.97 (1.0)

Example 5.2. *The optimal control problem* (1.4)-(1.5) *in two-dimensional case is considered with* $\Omega = (0,1)^2,\ T = 1,\ \gamma = 1,\ V(x_1, x_2) = x_1 + x_2$ *and* $\rho = 1$. *We set the exact solutions as*

$$\begin{aligned} u &= e^{-t\rho(x_1+x_2)} t x_1(1-x_1)x_2(1-x_2), \\ z &= e^{t\rho(x_1+x_2)}(1-t)x_1(1-x_1)x_2(1-x_2), \\ q &= \max\{-0.1, \min\{-z, -0.01\}\}, \end{aligned}$$

and evaluate f *and* u_d *by* (2.10), (2.11) *and the exact solutions.*

In Example 5.2, we choose $\tau = 1/8, 1/16, 1/32, 1/64$ to solve the problem (3.4)-(3.5) with $\alpha = 0.2, 0.5, 0.8$, and the domain $\Omega = (0,1)^2$ is partitioned into a uniform symmetric finite element triangulation mesh with the mesh size $h = 1/32$. The errors $|||\mathbf{u}-\mathbf{U}|||$, $|||\mathbf{z}-\mathbf{Z}|||$ and $|||\mathbf{q}-\mathbf{Q}|||$ are list in Table 3 together with numerical convergence orders in time direction, where a first order convergence order is shown. From the numerical results, we observe that our numerical scheme is efficient, the numerical convergence order is also not affected by the fractional order α, and the numerical results confirm the theoretical analysis in Theorem 4.1 as well. In Table 4, the $\ell^\infty(L^2(\Omega))$ errors and the corresponding numerical convergence orders are presented for Example 5.2, which shows the similar observations as in one dimensional case.

Table 3: The $\ell^2(L^2(\Omega))$ errors and numerical convergence orders for Example 5.2.

α	$\ell^2(L^2(\Omega))$ error	$\tau = 1/8$	$\tau = 1/16$	$\tau = 1/32$	$\tau = 1/64$	Order
0.2	$\|\|\|\mathbf{u}-\mathbf{U}\|\|\|$	3.36e-04	1.69e-04	8.31e-05	4.00e-05	$\approx$ 1.02 (1.0)
	$\|\|\|\mathbf{z}-\mathbf{Z}\|\|\|$	1.12e-03	5.54e-04	2.65e-04	1.20e-04	$\approx$ 1.08 (1.0)
	$\|\|\|\mathbf{q}-\mathbf{Q}\|\|\|$	1.10e-03	5.09e-04	2.41e-04	1.06e-04	$\approx$ 1.12 (1.0)
0.5	$\|\|\|\mathbf{u}-\mathbf{U}\|\|\|$	3.95e-04	2.00e-04	9.96e-05	4.95e-05	$\approx$ 1.00 (1.0)
	$\|\|\|\mathbf{z}-\mathbf{Z}\|\|\|$	1.09e-03	5.52e-04	2.73e-04	1.34e-04	$\approx$ 1.01 (1.0)
	$\|\|\|\mathbf{q}-\mathbf{Q}\|\|\|$	1.02e-03	4.46e-04	2.18e-04	1.05e-04	$\approx$ 1.09 (1.0)
0.8	$\|\|\|\mathbf{u}-\mathbf{U}\|\|\|$	6.23e-04	3.19e-04	1.62e-04	8.16e-05	$\approx$ 0.98 (1.0)
	$\|\|\|\mathbf{z}-\mathbf{Z}\|\|\|$	1.61e-03	8.35e-04	4.30e-04	2.25e-04	$\approx$ 0.95 (1.0)
	$\|\|\|\mathbf{q}-\mathbf{Q}\|\|\|$	1.49e-03	7.14e-04	3.69e-04	1.94e-04	$\approx$ 0.98 (1.0)

Table 4: The $\ell^\infty(L^2(\Omega))$ errors and numerical convergence orders for Example 5.2.

α	$\ell^\infty(L^2(\Omega))$ error	$\tau = 1/8$	$\tau = 1/16$	$\tau = 1/32$	$\tau = 1/64$	Order
0.2	$\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))}$	5.00e-04	2.99e-04	1.62e-04	8.32e-05	$\approx$ 0.86 (1.0)
	$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}$	1.52e-03	8.35e-04	4.64e-04	2.42e-04	$\approx$ 0.88 (1.0)
	$\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))}$	1.52e-03	7.43e-04	3.52e-04	1.55e-04	$\approx$ 1.10 (1.0)
0.5	$\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))}$	7.81e-04	4.23e-04	2.11e-04	1.04e-04	$\approx$ 0.97 (1.0)
	$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}$	2.14e-03	1.20e-03	6.13e-04	3.02e-04	$\approx$ 0.94 (1.0)
	$\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))}$	1.87e-03	8.69e-04	4.23e-04	2.16e-04	$\approx$ 1.04 (1.0)
0.8	$\|\mathbf{u}-\mathbf{U}\|_{\ell^\infty(L^2(\Omega))}$	1.08e-03	5.53e-04	2.85e-04	1.44e-04	$\approx$ 0.97 (1.0)
	$\|\mathbf{z}-\mathbf{Z}\|_{\ell^\infty(L^2(\Omega))}$	3.03e-03	1.55e-03	8.13e-04	4.18e-04	$\approx$ 0.95 (1.0)
	$\|\mathbf{q}-\mathbf{Q}\|_{\ell^\infty(L^2(\Omega))}$	2.58e-03	1.38e-03	7.12e-04	3.64e-04	$\approx$ 0.94 (1.0)

6 Conclusion

The forward fractional Feynman-Kac equation governs the joint probability density function of functionals in anomalous diffusion. This paper analyzes and approximates an optimal control problem governed by the forward fractional Feynman-Kac equation by a temporal semi-discrete scheme. Significant challenges are encountered in the theoretical analysis due to the time-space coupled nonlocal fractional substantial derivative in the equation. We establish the well-posedness, optimality conditions and solution regularity of the problem. Then we discretize the Riemann-Liouville fractional substantial derivative in time by using the backward Euler convolution quadrature formula and propose a temporal semi-discrete scheme for the optimal control problem. Based on the regularity results of the solution, we rigorously estimate the $\ell^2(L^2(\Omega))$ and $\ell^\infty(L^2(\Omega))$ discretization errors in time, and the theoretical convergence order of $O(\tau)$ is verified by some numerical examples. Due to the challenges as mentioned, the error analysis of the finite element method in space for the considered optimal control problem still confronts many difficulties.

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