

Error analysis of Crank-Nicolson scheme for an optimal control problem with time-fractional diffusion equation*

Xiaoyu Chen[†]

Wenyi Tian[‡]

Abstract

In this paper, an optimal control problem governed by a time-fractional diffusion equation is meticulously approximated based on Crank-Nicolson discretization in time to achieve higher temporal convergence order. Under absent control constraints, the regularity results on the second-order time derivatives of the control, state and adjoint variables in the optimality system are estimated. Together with the linear finite element discretization in space, we derive the optimality conditions of the discretized optimal control system and rigorously analyze the temporal error estimates of the control, state and adjoint variables only concerning the regularity property of the given data. The theoretical result indicates that our proposed Crank-Nicolson discretization scheme for the considered fractional optimal control problem converges by the optimal order of $O(\tau^{\min\{\frac{3}{2}+\alpha, 2\}})$ in time, which is verified in numerical examples.

Keywords: Optimal control, time-fractional diffusion equation, convolution quadrature, Crank-Nicolson scheme, finite element method, error estimate

AMS subject classifications: 35R11, 49M25, 65M12, 65M60

1 Introduction

Let Ω be a bounded convex polygonal domain with the boundary $\partial\Omega$ in \mathbb{R}^d , $d \geq 1$, and T be the fixed final time. This paper is dedicated to designing and analyzing a Crank-Nicolson scheme for an optimal control problem constrained by a time-fractional diffusion equation as follows

$$\min_{q \in U_{ad}} J(q) = \frac{1}{2} \|u(q) - u_d\|_{L^2(0,T;L^2(\Omega))}^2 + \frac{\gamma}{2} \|q\|_{L^2(0,T;L^2(\Omega))}^2 \quad (1.1)$$

with $u(q)$ determined by the time-fractional diffusion equation

$$\begin{cases} \partial_t u - \Delta \partial_t^{1-\alpha} u = f + q, & (x, t) \in \Omega \times (0, T], \\ u(x, t) = 0, & (x, t) \in \partial\Omega \times (0, T], \\ u(x, 0) = 0, & x \in \Omega, \end{cases} \quad (1.2)$$

where $\gamma > 0$ is a penalty parameter, $u_d : (0, T) \rightarrow L^2(\Omega)$ denotes the given target function, and the admissible set U_{ad} is given by

$$U_{ad} = \{q \in L^2(0, T; L^2(\Omega)) : a \leq q \leq b \text{ a.e. in } \Omega \times [0, T]\} \quad (1.3)$$

with $a, b \in \mathbb{R}$ and $a \leq b$. In (1.2), $f : (0, T) \rightarrow L^2(\Omega)$ is the given source term, the operator $\Delta : H_0^1(\Omega) \cap H^2(\Omega) \rightarrow L^2(\Omega)$ refers to the Dirichlet Laplacian, the notation $\partial_t^{1-\alpha}$ with $\alpha \in (0, 1)$ defined by

$$\partial_t^{1-\alpha} u(x, t) := \frac{1}{\Gamma(\alpha)} \frac{\partial}{\partial t} \int_0^t (t-s)^{\alpha-1} u(x, s) ds, \quad (1.4)$$

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[†]Center for Applied Mathematics and KL-AAGDM, Tianjin University, Tianjin 300072, China.

[‡]Corresponding author. Center for Applied Mathematics and KL-AAGDM, Tianjin University, Tianjin 300072, China (twymath@gmail.com).

represents the left-sided Riemann-Liouville fractional time derivative of order $(1 - \alpha)$, where $\Gamma(s) := \int_0^\infty t^{s-1} e^{-t} dt$ is the Euler gamma function [24].

In recent decades, investigations have revealed that the dynamics of numerous systems in physics, chemistry, and engineering can be more accurately described using fractional equations, as discussed in [19, 20, 24] and references therein. Anomalous diffusion, a widespread phenomenon in nature, has been observed in various fields, including solid surface diffusion [27], RNA movement in bacterial cytoplasm [2], ultracold atoms' anomalous diffusion in polarization optical lattice [26], animals' hunting strategy [25, 30], and so on. The time-fractional diffusion equation (1.2) has been extensively utilized to simulate anomalous diffusion phenomena in physics [19, 20, 33]. This equation describes a sublinear growth in the mean squared displacement of particle motion over time and has gained significant attention for its capability to depict anomalously slow diffusion processes, also known as subdiffusion. It is characterized by local motion occasionally interrupted by long sojourns and trapping effects. As the parameter α approaches 1, the equation (1.2) reduces to the classical diffusion equation, describing standard Brownian motion. The regularity of solutions to (1.2) has been well established in [14], and various numerical schemes for (1.2) have been designed and analyzed, as demonstrated in [6, 12, 16, 17, 15, 23, 37].

The optimal control problems governed by time fractional diffusion equations have attracted considerable interest in the past decade, both in theoretical issues and numerical algorithms [5, 9, 22, 21, 32, 34, 35, 36, 38, 39]. For an optimal control problem with constraint of the subdiffusion equation

$$\partial_t^\alpha u - \Delta u = f + q, \quad (1.5)$$

the existence, uniqueness, and first-order optimality condition were discussed with the control or state constraints in [21, 22]. In [34, 35], the authors developed a space-time spectral method for solving the optimal control problem constrained by the equation (1.5), and established the corresponding prior error estimates. The spatially semidiscrete Galerkin finite element scheme for the optimal control of (1.5) was proposed and analyzed in [38], and the temporal L1 discrete scheme was also considered without error estimates. Later, [9] estimated almost optimal-order convergence $O(\tau^\alpha)$ for the temporal discretization by L1 and backward Euler scheme. In [32], a piecewise constant discontinuous Galerkin method in time is considered and estimated.

The research on the optimal control problem (1.1)-(1.2) is relatively limited. In [39], the optimality system of the optimal control problem (1.1)-(1.2) was derived, and a piecewise constant time-stepping discontinuous Galerkin method combined with a piecewise linear finite element method was considered to solve the problem. In [5], the authors considered a fully discrete finite element method along with backward Euler convolution quadrature for time discretization, and estimated almost optimal convergence of $O(\tau |\ln \tau| + h^2)$. Nevertheless, the existing numerical schemes in aforementioned works only have first-order convergence, this motivates us to consider establishing a higher order scheme in time for solving the optimal control problem (1.1)-(1.2). Inspired by temporal discretization schemes with second order accuracy in [1, 18, 31] for parabolic optimal control problem, we will develop a Crank-Nicolson type scheme in time combining with the piecewise linear finite element in space for the optimal control problem (1.1)-(1.2). Then we derive the optimality system for the discretized optimal control problem, and rigorously analyze the error estimates without making additional assumptions about the regularity of the optimality system's solutions. The main result in Theorem 4.15 reveals that our proposed scheme for the problem (1.1)-(1.2) without control constraints has an optimal convergence order of $O(\tau^{\min\{\frac{3}{2}+\alpha, 2\}})$ in time.

The rest of this paper is organized as follows. We present some preliminaries and the semidiscrete scheme for the optimal control problem (1.1)-(1.2) based on the Galerkin finite element method in Section 2, and analyze the regularity estimates on the second derivatives of the control, state and adjoint variables with respect to time in the optimality system. In Section 3, we design a fully discrete scheme for the optimal control problem (1.1)-(1.2) by a Crank-Nicolson type discretization in time. Then the error estimates for temporal approximation are rigorously derived in Section 4. In Section 5, some numerical examples are illustrated to verify the theoretical convergence rates in temporal direction. Some conclusions are made in Section 6.

2 Preliminaries

In this section, we first state some main results on the optimality conditions, solutions representations and regularity for the optimal control problem (1.1)-(1.2), then present the spatial semidiscrete Galerkin finite element method for the problem and the error estimate derived in [5]. Throughout the paper, we denote $\|\cdot\|$ as the $L^2(\Omega)$ -norm, which induces the operator norm from $L^2(\Omega)$ to $L^2(\Omega)$, also denoted by $\|\cdot\|$.

2.1 Continuous problem

The adjoint derivative of $\partial_t^{1-\alpha}$ in (1.4) denoted by ${}^B\partial_t^{1-\alpha}$ is the $(1-\alpha)$ -th order right-sided Riemann-Liouville fractional derivative [24] with $\alpha \in (0, 1)$, and ${}^B\partial_t^{1-\alpha}z(x, t)$ is defined by

$${}^B\partial_t^{1-\alpha}z(x, t) := -\frac{1}{\Gamma(\alpha)}\frac{\partial}{\partial t}\int_t^T (s-t)^{\alpha-1}z(x, s)ds. \quad (2.1)$$

From [13, Lemma 2.3], the two types of Riemann-Liouville fractional derivatives in (1.4) and (2.1) satisfy the fractional integration by parts formula, that is

$$\int_0^T (\partial_t^{1-\alpha}u(t))z(t)dt = \int_0^T u(t)({}^B\partial_t^{1-\alpha}z(t))dt. \quad (2.2)$$

Lemma 2.1 ([5, 39]). *Let $q \in U_{ad}$ be the solution to the optimal control problem (1.1)-(1.2) and u the corresponding state variable given by (1.2). Then, there exists an adjoint state z such that (u, z, q) satisfies the optimality system*

$$\partial_t u - \Delta \partial_t^{1-\alpha}u = f + q, \quad \text{in } \Omega \times (0, T], \quad u = 0, \quad \text{on } \partial\Omega \times (0, T], \quad (2.3)$$

$$-\partial_t z - \Delta {}^B\partial_t^{1-\alpha}z = u - u_d, \quad \text{in } \Omega \times [0, T), \quad z = 0, \quad \text{on } \partial\Omega \times [0, T), \quad (2.4)$$

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

$$J'(q)(v - q) = \int_0^T \int_{\Omega} (\gamma q + z)(v - q)dxdt \geq 0, \quad \forall v \in U_{ad}. \quad (2.5)$$

The variational inequality (2.5) can be expressed as

$$q = P_{U_{ad}}\left(-\frac{1}{\gamma}z\right), \quad (2.6)$$

where $P_{U_{ad}}$ is a pointwise projection onto U_{ad} denoted by

$$P_{U_{ad}}(v(t)) = \max\{a, \min\{v(t), b\}\}, \quad (2.7)$$

one can refer to [11, 29, 40] for more details. We obtain from Lemma 2.1 that the objective functional $J(\cdot)$ in (1.1) is strongly convex, that is, the following property holds

$$J'(p)(p - q) - J'(q)(p - q) \geq \gamma\|p - q\|_{L^2(0,T;L^2(\Omega))}^2 \quad (2.8)$$

for any $p, q \in L^2(0, T; L^2(\Omega))$. This implies that the continuous optimal control problem (1.1)-(1.2) has a unique solution.

By using the Laplace transform, the solutions to (2.3) and (2.4) can be derived [5] as follows

$$u(\cdot, t) = \int_0^t E(t-s)(f(\cdot, s) + q(\cdot, s))ds, \quad (2.9)$$

$$z(\cdot, t) = \int_t^T E(s-t)(u(\cdot, s) - u_d(\cdot, s))ds, \quad (2.10)$$

where the operator $E(\cdot) : L^2(\Omega) \rightarrow L^2(\Omega)$ is given by

$$E(t) := \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t} \xi^{\alpha-1} (\xi^\alpha - \Delta)^{-1} d\xi, \quad (2.11)$$

with a contour $\Gamma_{\theta, \kappa}$ on the complex plane given by

$$\Gamma_{\theta, \kappa} = \{\xi \in \mathbb{C} : |\xi| = \kappa, |\arg \xi| \leq \theta\} \cup \{\xi \in \mathbb{C} : \xi = \rho e^{\pm i\theta}, \rho \geq \kappa\}. \quad (2.12)$$

The operator $E(\cdot) : L^2(\Omega) \rightarrow L^2(\Omega)$ in (2.11) can also be represented by

$$E(t)v = \sum_{j=1}^{\infty} E_{\alpha,1}(-\lambda_j t^\alpha)(v, \varphi_j) \varphi_j, \quad (2.13)$$

where $E_{\alpha,1}(\cdot)$ is the Mittag-Leffler function [24].

The following regularity of the solutions has been proved in [5, Lemma 2.4].

Lemma 2.2 ([5]). *Let (u, z, q) denote solutions of the system (2.3)-(2.5). For $f \in L^2(0, T; L^2(\Omega))$ and $u_d \in L^2(0, T; L^2(\Omega))$, we have*

$$\|u\|_{H^1(0, T; L^2(\Omega))} + \|u\|_{L^2(0, T; H^2(\Omega))} \leq C\|f + q\|_{L^2(0, T; L^2(\Omega))}, \quad (2.14)$$

$$\|z\|_{H^1(0, T; L^2(\Omega))} + \|z\|_{L^2(0, T; H^2(\Omega))} \leq C\|u - u_d\|_{L^2(0, T; L^2(\Omega))}, \quad (2.15)$$

$$\|q\|_{H^1(0, T; L^2(\Omega))} \leq C. \quad (2.16)$$

More regularity requirements are necessary to achieve more than first order convergence of temporal discrete schemes for the optimal control problem. We introduce the space $\dot{H}^p(\Omega) \subset L^2(\Omega)$ for $p \geq 0$ with the norm $\|v\|_{\dot{H}^p(\Omega)}^2 := \sum_{j=1}^{\infty} \lambda_j^p (v, \varphi_j)^2$, where $\{(\lambda_j, \varphi_j)\}_{j=1}^{\infty}$ are the L^2 -orthonormal eigenpairs of $-\Delta$ in Ω with a homogeneous Dirichlet boundary condition [28], in particular, $\dot{H}^0(\Omega) = L^2(\Omega)$, $\dot{H}^1(\Omega) = H_0^1(\Omega)$ and $\dot{H}^2(\Omega) = H^2(\Omega) \cap H_0^1(\Omega)$. With additional assumptions of f and u_d , we can obtain the following regularity results for the problem (2.3)-(2.5) with the admissible set $U_{ad} = L^2(0, T; L^2(\Omega))$.

Theorem 2.3. *Let (u, z, q) denote solutions of the system (2.3)-(2.5) with the admissible set $U_{ad} = L^2(0, T; L^2(\Omega))$. For $f \in H^2(0, T; \dot{H}^p(\Omega))$, $u_d \in H^2(0, T; \dot{H}^p(\Omega))$, $f(0) \in \dot{H}^{p+2}(\Omega)$, $f'(0) \in \dot{H}^p(\Omega)$, $u_d(T) \in \dot{H}^{p+2}(\Omega)$, $u_d'(T) \in \dot{H}^p(\Omega)$, $0 \leq p \leq 1$ and $\frac{1}{2} < \alpha < 1$, we have*

$$\|\partial_t^2 u\|_{L^2(0, T; \dot{H}^p(\Omega))} \leq C(\|g(0)\|_{\dot{H}^{p+2}(\Omega)} + \|g'(0)\|_{\dot{H}^p(\Omega)} + \|\partial_t^2 g\|_{L^2(0, T; \dot{H}^p(\Omega))}), \quad (2.17)$$

$$\|\partial_t^2 z\|_{L^2(0, T; \dot{H}^p(\Omega))} \leq C(\|\tilde{u}(T)\|_{\dot{H}^{p+2}(\Omega)} + \|\tilde{u}'(T)\|_{\dot{H}^p(\Omega)} + \|\partial_t^2 \tilde{u}\|_{L^2(0, T; \dot{H}^p(\Omega))}), \quad (2.18)$$

$$\|\partial_t^2 q\|_{L^2(0, T; \dot{H}^p(\Omega))} \leq C, \quad (2.19)$$

where $g(t) := f(t) + q(t)$ and $\tilde{u}(t) := u(t) - u_d(t)$.

Proof. By using (2.9) and (2.13), it obtains that

$$\begin{aligned} & \|\partial_t^2 u\|_{L^2(0, T; \dot{H}^p(\Omega))}^2 \\ &= \int_0^T \sum_{j=1}^{\infty} \lambda_j^p \left| \partial_t^2 \int_0^t E_{\alpha,1}(-\lambda_j(t-s)^\alpha)(g(s), \varphi_j) ds \right|^2 dt \\ &\leq 3 \left(\sum_{j=1}^{\infty} \lambda_j^p (g(0), \varphi_j)^2 \int_0^T (\partial_t E_{\alpha,1}(-\lambda_j t^\alpha))^2 dt + \sum_{j=1}^{\infty} \lambda_j^p (g'(0), \varphi_j)^2 \int_0^T (E_{\alpha,1}(-\lambda_j t^\alpha))^2 dt \right) \end{aligned}$$

$$\begin{aligned}
& + \sum_{j=1}^{\infty} \lambda_j^p \int_0^T \left(\int_0^t E_{\alpha,1}(-\lambda_j(t-s)^\alpha) (\partial_s^2 g(s), \varphi_j) ds \right)^2 dt \\
& = 3(I_1 + I_2 + I_3).
\end{aligned}$$

It indicates in [10, Lemma 1.3] that the Mittag-Leffler functions satisfy $\partial_t E_{\alpha,1}(-\lambda t^\alpha) = -\lambda t^{\alpha-1} E_{\alpha,\alpha}(-\lambda t^\alpha)$ and $|E_{\alpha,\alpha}(z)| \leq C/(1+|z|^2)$, then for $\alpha \in (1/2, 1)$, we derive that

$$\begin{aligned}
I_1 &= \sum_{j=1}^{\infty} \lambda_j^p (g(0), \varphi_j)^2 \int_0^T (-\lambda_j t^{\alpha-1} E_{\alpha,\alpha}(-\lambda_j t^\alpha))^2 dt \\
&\leq C \sum_{j=1}^{\infty} \lambda_j^p (g(0), \varphi_j)^2 \int_0^T \frac{\lambda_j^2 t^{2\alpha-2}}{(1+\lambda_j^2 t^{2\alpha})^2} dt \\
&\leq C \sum_{j=1}^{\infty} \lambda_j^{p+2} (g(0), \varphi_j)^2 = C \|g(0)\|_{\dot{H}^{p+2}(\Omega)}^2,
\end{aligned}$$

and $I_2 \leq C \|g'(0)\|_{\dot{H}^p(\Omega)}^2$ by the estimate $|E_{\alpha,1}(z)| \leq C/(1+|z|)$ in [10, Lemma 1.3]. In addition, it follows from Young's inequality for convolution that

$$\begin{aligned}
I_3 &= \sum_{j=1}^{\infty} \lambda_j^p \int_0^T \left(\int_0^t E_{\alpha,1}(-\lambda_j(t-s)^\alpha) (\partial_s^2 g(s), \varphi_j) ds \right)^2 dt \\
&\leq \sum_{j=1}^{\infty} \lambda_j^p \left(\int_0^T E_{\alpha,1}(-\lambda_j t^\alpha) dt \right)^2 \int_0^T (\partial_t^2 g(t), \varphi_j)^2 dt \\
&\leq C \|\partial_t^2 g\|_{L^2(0,T;\dot{H}^p(\Omega))}^2.
\end{aligned}$$

Thus, the estimate (2.17) is obtained. By the similar approach, (2.18) can also be derived by setting $p(\cdot, r) = z(\cdot, T-r)$ with $p(r)$ satisfying $\partial_r p(r) - \Delta \partial_r^{1-\alpha} p(r) = u(T-r) - u_d(T-r)$. Then it further deduces (2.19) from (2.6) and the condition $U_{ad} = L^2(0, T; L^2(\Omega))$. \square

Remark 2.4. If $f \in H^1(0, T; \dot{H}^p(\Omega))$, $u_d \in H^1(0, T; \dot{H}^p(\Omega))$, $f(0) \in \dot{H}^{p+2}(\Omega)$ and $u_d(T) \in \dot{H}^{p+2}(\Omega)$, then the estimates in Theorem 2.3 also hold by the similar approach.

2.2 Semidiscrete Galerkin scheme

Let $X_h \subset H_0^1(\Omega)$ be a continuous piecewise linear finite element space on a regular triangulation mesh \mathcal{T}_h of the domain Ω with $h = \max_{T \in \mathcal{T}_h} \text{diam}(T)$ being the maximal diameter. In [5], the semidiscrete Galerkin scheme with variational discretization for the control variable is considered for the optimal control problem (1.1)-(1.2), that is to find $q_h \in U_{ad}$ such that

$$\min_{q_h \in U_{ad}} J(q_h) = \frac{1}{2} \|u_h - u_d\|_{L^2(0,T;L^2(\Omega))}^2 + \frac{\gamma}{2} \|q_h\|_{L^2(0,T;L^2(\Omega))}^2 \quad (2.20)$$

subject to

$$(\partial_t u_h, \chi_h) + (\nabla \partial_t^{1-\alpha} u_h, \nabla \chi_h) = (f + q_h, \chi_h), \quad \forall \chi_h \in X_h \quad (2.21)$$

with $u_h(\cdot, 0) = 0$, where the control variable q_h is discretized in a variational concept in [7]. The corresponding discrete optimality conditions are as follows

$$(\partial_t u_h, \chi_h) + (\nabla \partial_t^{1-\alpha} u_h, \nabla \chi_h) = (f + q_h, \chi_h), \quad \forall \chi_h \in X_h, \quad t \in (0, T], \quad (2.22)$$

$$-(\partial_t z_h, \chi_h) + (\nabla^B \partial_t^{1-\alpha} z_h, \nabla \chi_h) = (u_h - u_d, \chi_h), \quad \forall \chi_h \in X_h, \quad t \in [0, T), \quad (2.23)$$

with $u_h(\cdot, 0) = 0$, $z_h(\cdot, T) = 0$ and

$$\int_0^T \int_{\Omega} (\gamma q_h + z_h)(v_h - q_h) dx dt \geq 0, \quad \forall v_h \in U_{ad}, \quad (2.24)$$

which implies that

$$q_h = P_{U_{ad}} \left(-\frac{1}{\gamma} z_h \right). \quad (2.25)$$

Similarly by using the Laplace transform, the solutions to (2.22)-(2.23) can be represented by

$$u_h(\cdot, t) = \int_0^t E_h(t-s) (f(\cdot, s) + q_h(\cdot, s)) ds, \quad (2.26)$$

$$z_h(\cdot, t) = \int_t^T E_h(s-t) (u_h(\cdot, s) - u_d(\cdot, s)) ds, \quad (2.27)$$

where the operator $E_h(\cdot) : L^2(\Omega) \rightarrow X_h$ is given by

$$E_h(t) := \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t} \xi^{\alpha-1} (\xi^{\alpha} - \Delta_h)^{-1} P_h d\xi, \quad (2.28)$$

and $P_h : L^2(\Omega) \rightarrow X_h$ denotes the L^2 projection operator by

$$(P_h \varphi, \chi_h) = (\varphi, \chi_h), \quad \forall \varphi \in L^2(\Omega), \quad \chi_h \in X_h. \quad (2.29)$$

In (2.28), the discrete Laplacian $\Delta_h : X_h \rightarrow X_h$ is defined by

$$(\Delta_h \varphi_h, \phi_h) = -(\nabla \varphi_h, \nabla \phi_h), \quad \forall \varphi_h, \phi_h \in X_h,$$

and it satisfies the following estimates [3, Lemma 5].

Lemma 2.5 ([3]). *For any $\xi \in \Sigma_{\theta} := \{\xi \in \mathbb{C} \setminus \{0\} : |\arg \xi| \leq \theta\}$ with $\theta \in (0, \pi)$, we have the resolvent estimates*

$$\|(\xi - \Delta_h)^{-1}\| \leq C|\xi|^{-1}, \quad (2.30)$$

$$\|\Delta_h^{1-\gamma}(\xi - \Delta_h)^{-1}\| \leq C|\xi|^{-\gamma}, \quad \gamma \in [0, 1]. \quad (2.31)$$

The regularity of the solutions of the semidiscrete system (2.22)-(2.24) has also been presented in [5, Lemma 3.2].

Lemma 2.6 ([5]). *Let (u_h, z_h, q_h) denote solutions of the system (2.22)-(2.24). For $f \in L^2(0, T; L^2(\Omega))$ and $u_d \in L^2(0, T; L^2(\Omega))$, we have*

$$\|u_h\|_{H^1(0, T; L^2(\Omega))} + \|u_h\|_{L^2(0, T; H^1(\Omega))} \leq C\|f + q_h\|_{L^2(0, T; L^2(\Omega))}, \quad (2.32)$$

$$\|z_h\|_{H^1(0, T; L^2(\Omega))} + \|z_h\|_{L^2(0, T; H^1(\Omega))} \leq C\|u_h - u_d\|_{L^2(0, T; L^2(\Omega))}, \quad (2.33)$$

$$\|q_h\|_{H^1(0, T; L^2(\Omega))} \leq C. \quad (2.34)$$

Remark 2.7. *By the similar approach as in Theorem 2.3, analogous regularity estimates in $H^2(0, T; L^2(\Omega))$ can be established for the semidiscrete solutions (u_h, z_h, q_h) of the system (2.22)-(2.24).*

In [5, Theorem 3.1], the optimal finite element error estimates in space are derived for the semidiscrete system (2.22)-(2.24).

Theorem 2.8 ([5]). *Let (u, z, q) and (u_h, z_h, q_h) be the solutions of the systems (2.3)-(2.5) and (2.22)-(2.24), respectively. For $f \in L^2(0, T; L^2(\Omega))$ and $u_d \in L^2(0, T; L^2(\Omega))$, we have*

$$\|u - u_h\|_{L^2(0, T; L^2(\Omega))} + \|z - z_h\|_{L^2(0, T; L^2(\Omega))} + \|q - q_h\|_{L^2(0, T; L^2(\Omega))} \leq Ch^2,$$

$$\|\nabla(u - u_h)\|_{L^2(0, T; L^2(\Omega))} + \|\nabla(z - z_h)\|_{L^2(0, T; L^2(\Omega))} \leq Ch,$$

where the constant C is independent of h .

3 Fully discrete Crank-Nicolson scheme

In this section, we devote to designing the fully discrete numerical discretization with Crank-Nicolson scheme in time for the optimal control problem (1.1)-(1.2).

The time interval $[0, T]$ is divided into a uniform partition with a step size $\tau = T/N$, and $t_n = n\tau$, $n = 0, \dots, N$. We denote $\bar{\partial}_\tau^{1-\alpha}$ the Grünwald-Letnikov difference formula (also called the backward Euler convolution quadrature) by

$$\bar{\partial}_\tau^{1-\alpha} U_h^n := \frac{1}{\tau^{1-\alpha}} \sum_{j=1}^n b_{n-j} U_h^j, \quad n = 1, 2, \dots, N, \quad (3.1)$$

where the coefficients $\{b_j, j \geq 0\}$ satisfy the following power series expansion

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

and the recursive formula $b_0 = 1$, $b_j = b_{j-1} \cdot \frac{\alpha+j-2}{j}$, $j = 1, 2, \dots$. The notation $\bar{\partial}_\tau^{1-\alpha}$ in (3.1) reduces to the standard backward Euler difference operator $\bar{\partial}_\tau$ when $\alpha = 0$ and

$$\bar{\partial}_\tau U_h^n := \frac{U_h^n - U_h^{n-1}}{\tau}, \quad n = 1, 2, \dots, N. \quad (3.3)$$

By using the approach in [6], the time-fractional derivative at $t_n - \frac{\tau}{2}$ can be approximated by

$$\begin{aligned} \partial_t^{1-\alpha} u_h(t_n - \frac{\tau}{2}) &= (1 - \frac{\alpha}{2}) \partial_t^{1-\alpha} u_h(t_n - \frac{1-\alpha}{2} \tau) + \frac{\alpha}{2} \partial_t^{1-\alpha} u_h(t_{n-1} - \frac{1-\alpha}{2} \tau) + O(\tau^2) \\ &= (1 - \frac{\alpha}{2}) \bar{\partial}_\tau^{1-\alpha} u_h^n + \frac{\alpha}{2} \bar{\partial}_\tau^{1-\alpha} u_h^{n-1} + O(\tau^2), \end{aligned}$$

then we obtain a fully discrete Crank-Nicolson scheme for (1.2) as follows

$$\bar{\partial}_\tau U_h^n - (1 - \frac{\alpha}{2}) \Delta_h \bar{\partial}_\tau^{1-\alpha} U_h^n - \frac{\alpha}{2} \Delta_h \bar{\partial}_\tau^{1-\alpha} U_h^{n-1} = f_h^{n-\frac{1}{2}} + P_h q_h^{n-\frac{1}{2}} \quad (3.4)$$

for $n = 1, 2, \dots, N$, with $U_h^0 = 0$, $f_h^{n-\frac{1}{2}} = P_h f(x, t_{n-\frac{1}{2}})$ and $q_h^{n-\frac{1}{2}} = q_h(x, t_{n-\frac{1}{2}})$, where P_h is the L^2 projection operator given by (2.29). Note that the fully discrete scheme (3.4) for (1.2) with the averaged values of right terms at t_n and t_{n-1} is different from that in [6], and such modification makes the scheme (3.4) become applicable for approximating the optimal control problem (1.1)-(1.2).

We propose the fully discrete Crank-Nicolson scheme for the optimal control problem (1.1)-(1.2) as follows

$$\min_{\mathbf{Q}_h \in U_{ad}^\tau} J_\tau(\mathbf{Q}_h) = \frac{\tau}{4} \|U_h^0 - u_d^0\|^2 + \frac{\tau}{2} \sum_{n=1}^{N-1} \|U_h^n - u_d^n\|^2 + \frac{\tau}{4} \|U_h^N - u_d^N\|^2 + \frac{\tau}{2} \sum_{n=1}^N \gamma \|Q_h^{n-\frac{1}{2}}\|^2 \quad (3.5)$$

subject to

$$\bar{\partial}_\tau U_h^n - (1 - \frac{\alpha}{2}) \Delta_h \bar{\partial}_\tau^{1-\alpha} U_h^n - \frac{\alpha}{2} \Delta_h \bar{\partial}_\tau^{1-\alpha} U_h^{n-1} = f_h^{n-\frac{1}{2}} + P_h Q_h^{n-\frac{1}{2}} \quad (3.6)$$

for $n = 1, 2, \dots, N$, with $U_h^0 = 0$, $f_h^{n-\frac{1}{2}} = P_h f(x, t_{n-\frac{1}{2}})$ and $Q_h^{n-\frac{1}{2}} = Q_h(x, t_{n-\frac{1}{2}})$. The discrete admissible set U_{ad}^τ in (3.5) is

$$U_{ad}^\tau = \{\mathbf{Q}_h = (Q_h^{n-\frac{1}{2}})_{n=1}^N : a \leq Q_h^{n-\frac{1}{2}} \leq b, n = 1, 2, \dots, N\}.$$

Let the notations ${}^B\bar{\partial}_\tau^{1-\alpha}Z_h^{n-\frac{1}{2}}$ and ${}^B\bar{\partial}_\tau Z_h^{n-\frac{1}{2}}$ be defined by

$${}^B\bar{\partial}_\tau^{1-\alpha}Z_h^{n-\frac{1}{2}} := \frac{1}{\tau^{1-\alpha}} \sum_{j=n}^N b_{j-n} Z_h^{j-\frac{1}{2}}, \quad {}^B\bar{\partial}_\tau Z_h^{n-\frac{1}{2}} := \frac{Z_h^{n-\frac{1}{2}} - Z_h^{n+\frac{1}{2}}}{\tau}, \quad n = 1, 2, \dots, N,$$

respectively, we can obtain by the above notations and simple calculations that

$$\tau \sum_{n=1}^N (Z_h^{n-\frac{1}{2}}, \bar{\partial}_\tau U_h^n) = \tau \sum_{n=1}^{N-1} ({}^B\bar{\partial}_\tau Z_h^{n-\frac{1}{2}}, U_h^n) + (U_h^N, Z_h^{N-\frac{1}{2}}) - (U_h^0, Z_h^{\frac{1}{2}}), \quad (3.7)$$

$$\tau \sum_{n=1}^N ({}^B\bar{\partial}_\tau^{1-\alpha} Z_h^{n-\frac{1}{2}}, U_h^n) = \tau \sum_{n=1}^N (Z_h^{n-\frac{1}{2}}, \bar{\partial}_\tau^{1-\alpha} U_h^n), \quad (3.8)$$

$$\tau \sum_{n=1}^N ({}^B\bar{\partial}_\tau^{1-\alpha} Z_h^{n-\frac{1}{2}}, U_h^{n-1}) = \tau \sum_{n=1}^N (Z_h^{n-\frac{1}{2}}, \bar{\partial}_\tau^{1-\alpha} U_h^{n-1}). \quad (3.9)$$

3.1 Optimality conditions and solution representations

In this subsection, we derive the optimality conditions of the fully discrete optimal control problem (3.5)-(3.6) with Crank-Nicolson scheme, and then investigate integral representations of the solutions and their stability analysis. We introduce the following notations for further discussions.

$$\begin{aligned} \mathbf{u}_h &= (u_h(\cdot, t_n))_{n=1}^N, & \mathbf{z}_h &= (z_h(\cdot, t_{n-\frac{1}{2}}))_{n=1}^N, & \mathbf{q}_h &= (q_h(\cdot, t_{n-\frac{1}{2}}))_{n=1}^N, \\ \mathbf{U}_h &= (U_h^n)_{n=1}^N, & \mathbf{Z}_h &= (Z_h^{n-\frac{1}{2}})_{n=1}^N, & \mathbf{Q}_h &= (Q_h^{n-\frac{1}{2}})_{n=1}^N. \end{aligned}$$

The discrete space-time inner product and norm are defined by

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

Theorem 3.1. *The fully discrete optimal control problem (3.5)-(3.6) admits a unique solution $(\mathbf{U}_h, \mathbf{Q}_h)$ and an adjoint state \mathbf{Z}_h such that $(\mathbf{U}_h, \mathbf{Q}_h, \mathbf{Z}_h)$ satisfies the following optimality system*

$$\bar{\partial}_\tau U_h^n - (1 - \frac{\alpha}{2}) \Delta_h \bar{\partial}_\tau^{1-\alpha} U_h^n - \frac{\alpha}{2} \Delta_h \bar{\partial}_\tau^{1-\alpha} U_h^{n-1} = f_h^{n-\frac{1}{2}} + P_h Q_h^{n-\frac{1}{2}}, \quad n = 1, \dots, N, \quad (3.10)$$

$$\begin{cases} \frac{Z_h^{N-\frac{1}{2}}}{\tau} - (1 - \frac{\alpha}{2}) \Delta_h {}^B\bar{\partial}_\tau^{1-\alpha} Z_h^{N-\frac{1}{2}} = \frac{U_h^N - P_h u_d^N}{2}, \\ {}^B\bar{\partial}_\tau Z_h^{n-\frac{1}{2}} - (1 - \frac{\alpha}{2}) \Delta_h {}^B\bar{\partial}_\tau^{1-\alpha} Z_h^{n-\frac{1}{2}} - \frac{\alpha}{2} \Delta_h {}^B\bar{\partial}_\tau^{1-\alpha} Z_h^{n+\frac{1}{2}} = U_h^n - P_h u_d^n, \end{cases} \quad (3.11)$$

for $n = N-1, \dots, 1$, and

$$(\gamma Q_h^{n-\frac{1}{2}} + Z_h^{n-\frac{1}{2}}, W - Q_h^{n-\frac{1}{2}}) \geq 0, \quad \forall W \in U_{ad}^\tau. \quad (3.12)$$

Proof. By the strong convexity of the fully discrete optimal control problem (3.5)-(3.6), it admits a unique solution $(\mathbf{U}_h, \mathbf{Q}_h)$.

Due to the convexity of U_{ad}^τ , it holds that $\mathbf{Q}_h + \varepsilon \delta \mathbf{Q}_h \in U_{ad}^\tau$ with $\delta \mathbf{Q}_h := \mathbf{W} - \mathbf{Q}_h$ for $0 < \varepsilon \ll 1$ and any $\mathbf{W} \in U_{ad}^\tau$. We have from (3.6) that $\delta U_h = \lim_{\varepsilon \rightarrow 0+} (U_h(\mathbf{Q}_h + \varepsilon \delta \mathbf{Q}_h) - U_h(\mathbf{Q}_h)) / \varepsilon$ satisfies the following variational form

$$(\bar{\partial}_\tau \delta U_h^n, \chi_h) + (1 - \frac{\alpha}{2}) (\nabla \bar{\partial}_\tau^{1-\alpha} \delta U_h^n, \nabla \chi_h) + \frac{\alpha}{2} (\nabla \bar{\partial}_\tau^{1-\alpha} \delta U_h^{n-1}, \nabla \chi_h) = (\delta Q_h^{n-\frac{1}{2}}, \chi_h). \quad (3.13)$$

By taking $\chi_h = Z_h^{n-\frac{1}{2}}$ in (3.13), it obtains from (3.7), (3.8), (3.9) and (3.11) that the differentiation of $J_\tau(\mathbf{Q}_h)$ is as follows

$$\begin{aligned}
0 &\leq \lim_{\varepsilon \rightarrow 0^+} \frac{J_\tau(\mathbf{Q}_h + \varepsilon \delta \mathbf{Q}_h) - J_\tau(\mathbf{Q}_h)}{\varepsilon} \\
&= \frac{\tau}{2} \int_{\Omega} (U_h^N(\mathbf{Q}_h) - u_d^N) \delta U_h^N dx + \tau \sum_{n=1}^{N-1} \int_{\Omega} (U_h^n(\mathbf{Q}_h) - u_d^n) \delta U_h^n dx \\
&\quad + \tau \sum_{n=1}^N \int_{\Omega} \gamma Q_h^{n-\frac{1}{2}} \delta Q_h^{n-\frac{1}{2}} dx \\
&= \tau \sum_{n=1}^N \int_{\Omega} (\gamma Q_h^{n-\frac{1}{2}} + Z_h^{n-\frac{1}{2}}) \delta Q_h^{n-\frac{1}{2}} dx.
\end{aligned}$$

Thus the proof is completed. \square

We next derive the representations of the solutions to the system (3.10)-(3.12) by using Cauchy's integral formula and analyze their stability estimates. The truncated contour $\Gamma_{\theta, \kappa}^\tau$ of $\Gamma_{\theta, \kappa}$ in (2.12) is defined by

$$\Gamma_{\theta, \kappa}^\tau = \{z \in \Gamma_{\theta, \kappa} : |\operatorname{Im}(\xi)| \leq \frac{\pi}{\tau}\}. \quad (3.14)$$

Theorem 3.2. *Let $G_h^n := f_h^{n-\frac{1}{2}} + P_h Q_h^{n-\frac{1}{2}}$ and $M_h^n := U_h^n - P_h u_d^n$. The solutions of the fully discrete scheme (3.10)-(3.11) can be represented as*

$$\begin{aligned}
U_h^n &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \beta_\tau(e^{-\xi\tau})^\alpha [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} \tilde{G}_h(e^{-\xi\tau}) d\xi, \\
&= \tau \sum_{k=1}^n E_\tau^{n-k} (f_h^{k-\frac{1}{2}} + Q_h^{k-\frac{1}{2}}),
\end{aligned} \quad (3.15)$$

$$\begin{aligned}
Z_h^{n-\frac{1}{2}} &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi(T-t_n)} \beta_\tau(e^{-\xi\tau})^\alpha [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} \tilde{M}_h(e^{-\xi\tau}) d\xi, \\
&= \frac{1}{2} \tau E_\tau^{N-n} (U_h^N - u_d^N) + \tau \sum_{k=1}^{N-n} E_\tau^{N-n-k} (U_h^{N-k} - u_d^{N-k}),
\end{aligned} \quad (3.16)$$

where the operators $E_\tau^n : L^2(\Omega) \rightarrow X_h$ are given by

$$E_\tau^n = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \beta_\tau(e^{-\xi\tau})^\alpha [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} P_h d\xi, \quad (3.17)$$

and the functions $\delta_\tau(\cdot)$, $\beta_\tau(\cdot)$, $\tilde{G}_h(\cdot)$ and $\tilde{M}_h(\cdot)$ are respectively given by

$$\delta_\tau(\zeta) = \frac{1-\zeta}{\tau}, \quad \beta_\tau(\zeta) = \frac{\delta_\tau(\zeta)}{(1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta)^{\frac{1}{\alpha}}}, \quad (3.18)$$

$$\tilde{G}_h(\zeta) = \sum_{n=0}^{\infty} G_h^n \zeta^n, \quad \tilde{M}_h(\zeta) = \sum_{n=-\infty}^N M_h^n \zeta^{N-n} - \frac{1}{2} M_h^N, \quad (3.19)$$

Proof. Multiplying (3.10) by ζ^n on both sides and summing n from 1 to ∞ yields

$$\tilde{U}_h(\zeta) := \sum_{n=0}^{\infty} U_h^n \zeta^n = \delta_\tau(\zeta)^{\alpha-1} \left[\frac{\delta_\tau(\zeta)^\alpha}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta} - \Delta_h \right]^{-1} \frac{\tilde{G}_h(\zeta)}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta}. \quad (3.20)$$

Then it further follows that

$$\begin{aligned} U_h^n &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \delta_\tau(e^{-\xi\tau})^{\alpha-1} \left[\frac{\delta_\tau(e^{-\xi\tau})^\alpha}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}e^{-\xi\tau}} - \Delta_h \right]^{-1} \frac{\tilde{G}_h(e^{-\xi\tau})}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}e^{-\xi\tau}} d\xi \\ &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \beta_\tau(e^{-\xi\tau})^\alpha [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} \tilde{G}_h(e^{-\xi\tau}) d\xi, \end{aligned} \quad (3.21)$$

which confirms the first equality of (3.15).

By changing the variable $\zeta = e^{-\xi\tau}$, it also yields that

$$\begin{aligned} \tau E_\tau^n &:= \frac{1}{2\pi i} \int_{|\zeta|=\rho} \zeta^{-n-1} \left[\frac{\delta_\tau(\zeta)^\alpha}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta} - \Delta_h \right]^{-1} \frac{\delta_\tau(\zeta)^{\alpha-1}}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta} P_h d\zeta \\ &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \beta_\tau(e^{-\xi\tau})^\alpha [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} P_h d\xi. \end{aligned} \quad (3.22)$$

Hence, we derive from (3.20) and Cauchy's integral formula that

$$\tilde{U}_h(\zeta) = \left(\sum_{n=0}^{\infty} \tau E_\tau^n \zeta^n \right) \left(\sum_{n=1}^{\infty} (f_h^{n-\frac{1}{2}} + Q_h^{n-\frac{1}{2}}) \zeta^n \right),$$

and the coefficients of the power series on both sides lead to the second equality of (3.15).

By the similar approach, we can obtain the solution representation for (3.11). It obtains by multiplying ζ^{N-n} on both sides of (3.11) and summing n from $-\infty$ to N that

$$\tilde{Z}_h(\zeta) := \sum_{n=-\infty}^N Z_h^{n-\frac{1}{2}} \zeta^{N-n} = \delta_\tau(\zeta)^{\alpha-1} \left[\frac{\delta_\tau(\zeta)^\alpha}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta} - \Delta_h \right]^{-1} \frac{\widetilde{M}_h(\zeta)}{1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta}, \quad (3.23)$$

which is analytic with respect to ζ in a neighborhood of the origin. Then applying Cauchy's integral formula implies that

$$\begin{aligned} Z_h^{n-\frac{1}{2}} &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi(T-t_n)} \tilde{Z}_h(e^{-\xi\tau}) d\xi \\ &= \frac{\tau}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi(T-t_n)} \beta_\tau(e^{-\xi\tau})^\alpha [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} \widetilde{M}_h(e^{-\xi\tau}) d\xi, \end{aligned} \quad (3.24)$$

which obtains the first equality of (3.16). Similarly, it has from (3.23) and (3.22) that

$$\tilde{Z}_h(\zeta) = \left(\sum_{n=-\infty}^N \tau E_\tau^{N-n} \zeta^{N-n} \right) \left(\sum_{n=-\infty}^N \frac{1}{2} (U_h^n - u_d^n) \zeta^{N-n} + \sum_{n=-\infty}^N \frac{1}{2} (U_h^{n-1} - u_d^{n-1}) \zeta^{N-n+1} \right).$$

Thus, the second equality of (3.16) is obtained by comparing the coefficients of the power series on both sides of the above formula. \square

The functions $\delta_\tau(\cdot)$ and $\beta_\tau(\cdot)$ in (3.18) satisfy the properties in the following two lemmas, which are derived in [4, Lemma 3.4] and [8, Lemmas 3.3 and 3.4], respectively.

Lemma 3.3 ([4]). *Let $\alpha \in (0, 1)$, $\theta \in (\frac{\pi}{2}, \operatorname{arccot}(-\frac{2}{\pi}))$ and $\delta_\tau(\cdot)$ be defined in (3.18). Then, for any $\xi \in \Gamma_{\theta, \kappa}^\tau$, we have $\delta_\tau(e^{-\xi\tau}) \in \Sigma_\theta$ and*

$$C_0 |\xi| \leq |\delta_\tau(e^{-\xi\tau})| \leq C_1 |\xi|, \quad (3.25)$$

$$|\delta_\tau(e^{-\xi\tau}) - \xi| \leq C\tau |\xi|^2, \quad (3.26)$$

$$|\delta_\tau(e^{-\xi\tau})^\alpha - \xi^\alpha| \leq C\tau |\xi|^{\alpha+1}, \quad (3.27)$$

where Σ_θ is defined in Lemma 2.5 and the constants C_0, C_1 and C are independent of τ and κ .

Lemma 3.4 ([8]). Let $\alpha \in (0, 1)$, $\phi \in (\alpha\pi/2, \pi)$ and $\beta_\tau(\cdot)$ be defined in (3.18). Then there exists a constant $\kappa_1 > 0$ (independent of τ) such that for $\kappa \in (0, \kappa_1]$, $\theta \in (\pi/2, \pi/2 + \kappa_1]$ and any $\xi \in \Gamma_{\theta, \kappa}^\tau$, we have $\beta_\tau(e^{-\xi\tau}) \in \Sigma_\phi$ and

$$C_0|\xi| \leq |\beta_\tau(e^{-\xi\tau})| \leq C_1|\xi|, \quad (3.28)$$

$$|\beta_\tau(e^{-\xi\tau}) - \xi| \leq C\tau^2|\xi|^3, \quad (3.29)$$

$$|\beta_\tau(e^{-\xi\tau})^\alpha - \xi^\alpha| \leq C\tau^2|\xi|^{2+\alpha}, \quad (3.30)$$

where the constants C_0, C_1 and C are independent of τ, θ and κ (but may depend on κ_1).

For the error analysis of the fully discrete optimal control problem (3.5)-(3.6) in the next section, we introduce three auxiliary notations $\mathbf{U}_h(\mathbf{q}_h)$, $\mathbf{Z}_h(\mathbf{U}_h(\mathbf{q}_h))$, $\mathbf{Z}_h(\mathbf{u}_h)$, which respectively satisfy the following three systems

$$\begin{cases} \bar{\partial}_\tau U_h(q_h)^n - (1 - \frac{\alpha}{2})\Delta_h \bar{\partial}_\tau^{1-\alpha} U_h(q_h)^n - \frac{\alpha}{2}\Delta_h \bar{\partial}_\tau^{1-\alpha} U_h(q_h)^{n-1} = f_h^{n-\frac{1}{2}} + P_h q_h^{n-\frac{1}{2}}, \\ U_h(q_h)^0 = 0, \quad n = 1, 2, \dots, N, \end{cases} \quad (3.31)$$

$$\begin{cases} \frac{Z_h(U_h(q_h))^{N-\frac{1}{2}}}{\tau} - (1 - \frac{\alpha}{2})\Delta_h^B \bar{\partial}_\tau^{1-\alpha} Z_h(U_h(q_h))^{N-\frac{1}{2}} = \frac{U_h(q_h)^N - P_h u_d^N}{2}, \\ {}^B \bar{\partial}_\tau Z_h(U_h(q_h))^{n-\frac{1}{2}} - (1 - \frac{\alpha}{2})\Delta_h^B \bar{\partial}_\tau^{1-\alpha} Z_h(U_h(q_h))^{n-\frac{1}{2}} - \frac{\alpha}{2}\Delta_h^B \bar{\partial}_\tau^{1-\alpha} Z_h(U_h(q_h))^{n+\frac{1}{2}} \\ = U_h(q_h)^n - P_h u_d^n, \end{cases} \quad (3.32)$$

$$\begin{cases} \frac{Z_h(u_h)^{N-\frac{1}{2}}}{\tau} - (1 - \frac{\alpha}{2})\Delta_h^B \bar{\partial}_\tau^{1-\alpha} Z_h(u_h)^{N-\frac{1}{2}} = \frac{u_h^N - P_h u_d^N}{2}, \\ {}^B \bar{\partial}_\tau Z_h(u_h)^{n-\frac{1}{2}} - (1 - \frac{\alpha}{2})\Delta_h^B \bar{\partial}_\tau^{1-\alpha} Z_h(u_h)^{n-\frac{1}{2}} - \frac{\alpha}{2}\Delta_h^B \bar{\partial}_\tau^{1-\alpha} Z_h(u_h)^{n+\frac{1}{2}} = u_h^n - P_h u_d^n, \end{cases} \quad (3.33)$$

for $n = N - 1, \dots, 1$.

In the following, we obtain the stability results of the solutions to (3.10), (3.11) and (3.31)-(3.33).

Theorem 3.5. Let U_h^n , $Z_h^{n-\frac{1}{2}}$, $U_h(q_h)^n$, $Z_h(U_h(q_h))^{n-\frac{1}{2}}$ and $Z_h(u_h)^{n-\frac{1}{2}}$ be solutions to (3.10), (3.11), (3.31), (3.32) and (3.33), respectively. Then we have

$$\|\mathbf{U}_h(\mathbf{q}_h) - \mathbf{U}_h\| \leq C\|\mathbf{q}_h - \mathbf{Q}_h\|, \quad (3.34)$$

$$\|\mathbf{Z}_h(\mathbf{U}_h(\mathbf{q}_h)) - \mathbf{Z}_h(\mathbf{u}_h)\| \leq C\|\mathbf{U}_h(\mathbf{q}_h) - \mathbf{u}_h\|, \quad (3.35)$$

$$\|\mathbf{Z}_h(\mathbf{u}_h) - \mathbf{Z}_h\| \leq C\|\mathbf{u}_h - \mathbf{U}_h\|, \quad (3.36)$$

where the constant C is independent of τ .

Proof. The operators E_τ^n in (3.17) are bounded by using Lemmas 2.5, 3.3 and 3.4, that is

$$\begin{aligned} \|E_\tau^n(t)\| &\leq C \int_{\Gamma_{\theta, \kappa}^\tau} |e^{\xi t}| |\beta_\tau(e^{-\xi\tau})|^\alpha \|[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\| |\delta_\tau(e^{-\xi\tau})^{-1}| |d\xi| \\ &\leq C \int_{\Gamma_{\theta, \kappa}^\tau} |e^{\xi t}| |\xi|^{-1} |d\xi| \leq C. \end{aligned}$$

Then it has from the expression (3.15) that

$$\|U_h(q_h)^n - U_h^n\| \leq \tau \sum_{k=1}^n \|E_\tau^{n-k}\| \|q_h^{k-\frac{1}{2}} - Q_h^{k-\frac{1}{2}}\| \leq C\tau \sum_{k=1}^n \|q_h^{k-\frac{1}{2}} - Q_h^{k-\frac{1}{2}}\|,$$

which directly implies (3.34) from

$$\|U_h(q_h) - U_h\|^2 \leq C\tau \sum_{n=1}^N \left(\tau \sum_{k=1}^N \|q_h^{k-\frac{1}{2}} - Q_h^{k-\frac{1}{2}}\| \right)^2 \leq C \|q_h - Q_h\|^2.$$

Next we consider the estimate (3.35). We have from (3.16) that

$$\begin{aligned} & \|Z_h(U_h(q_h))^{n-\frac{1}{2}} - Z_h(u_h)^{n-\frac{1}{2}}\|_{L^2(\Omega)} \\ & \leq \frac{1}{2}\tau \|E_\tau^{N-n}\| \|U_h(q_h)^N - u_h^N\| + \tau \sum_{k=1}^{N-n} \|E_\tau^{N-n-k}\| \|U_h(q_h)^{N-k} - u_h^{N-k}\| \\ & \leq C\tau \sum_{k=0}^{N-n} \|E_\tau^{N-n-k}\| \|U_h(q_h)^{N-k} - u_h^{N-k}\| \leq C\tau \sum_{k=n}^N \|U_h(q_h)^k - u_h^k\|. \end{aligned}$$

Then we further obtain that

$$\|Z_h(U_h(q_h)) - Z_h(u_h)\|^2 \leq C\tau \sum_{n=1}^N \left(\tau \sum_{k=1}^N \|U_h(q_h)^k - u_h^k\| \right)^2 \leq C \|U_h(q_h) - u_h\|^2.$$

By the similar approach as above, the estimate (3.36) can also be derived from (3.16). \square

4 Error estimates

In this section, we consider the analysis of temporal errors between the fully discrete Crank-Nicolson scheme (3.5)-(3.6) and the semidiscrete scheme (2.20)-(2.21) for the case of the admissible set $U_{ad} = L^2(0, T; L^2(\Omega))$, including the error estimates of $\|u_h - U_h\|$, $\|z_h - Z_h\|$ and $\|q_h - Q_h\|$. The main result is stated in Theorem 4.15.

We first consider the temporal error estimates of $\|u_h - U_h(q_h)\|$ and $\|z_h - Z_h(u_h)\|$ for the schemes (3.31) and (3.33), respectively, in the next two subsections. The following lemma is necessary for our analysis, which refers to [6, Lemma 3.2].

Lemma 4.1 ([6]). *Let $\alpha \in (0, 1)$, $\mu(\cdot)$ and $\gamma(\cdot)$ be defined by*

$$\mu(\zeta) = \frac{\zeta}{(1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta)^{\frac{2}{\alpha}}}, \quad \gamma(\zeta) = \frac{\frac{1}{2} + \frac{1}{2}\zeta}{(1 - \frac{\alpha}{2} + \frac{\alpha}{2}\zeta)^{\frac{1}{\alpha}}}. \quad (4.1)$$

Then there exists a constant $\kappa_1 > 0$ (independent of τ) such that for $\kappa \in (0, \kappa_1]$ and $\theta \in (\pi/2, \pi/2 + \kappa_1]$, it holds that

$$|\mu(e^{-\xi\tau})| \leq C, \quad |\gamma(e^{-\xi\tau})| \leq C, \quad (4.2)$$

$$|\mu(e^{-\xi\tau}) - 1| \leq C\tau^2|\xi|^2, \quad |\gamma(e^{-\xi\tau}) - 1| \leq C\tau^2|\xi|^2, \quad (4.3)$$

for any $\xi \in \Gamma_{\theta, \kappa}^\tau$, where the constants C are independent of τ, θ and κ (maybe dependent on κ_1).

4.1 Error estimate of $\|u_h - U_h(q_h)\|$

In this subsection, we derive the error estimate of $\|u_h - U_h(q_h)\|$ by analyzing the error $\|u_h(t_n) - U_h(q_h)^n\|$ for each term in the Taylor expansions of the source terms $f_h(t)$ and $q_h(t)$,

$$f_h(t) = f_h(0) + tf_h'(0) + (t * f_h'')(t), \quad q_h(t) = q_h(0) + tq_h'(0) + (t * q_h'')(t).$$

It shows that the estimate of $\|u_h(t_n) - U_h(q_h)^n\|$ consists of errors for three parts: $f_h(0)$ and $q_h(0)$; $tf_h'(0)$ and $tq_h'(0)$; $(t * f_h'')(t)$ and $(t * q_h'')(t)$.

For the case $f_h(t) = f_h(0)$ and $q_h(t) = q_h(0)$, it follows from (2.26) and Theorem 3.2 that the solutions $u_h(t_n)$ and $U_h(q_h)^n$ to (2.22) and (3.31) with $f_h(t) = f_h(0)$ and $q_h(t) = q_h(0)$ can be represented as

$$\begin{aligned} u_h(t_n) &= \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t_n} \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} (f_h(0) + P_h q_h(0)) d\xi \\ &= t_n (f_h(0) + P_h q_h(0)) + \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t_n} \xi^{-2} (\xi^\alpha - \Delta_h)^{-1} \Delta_h P_h (f(0) + q_h(0)) d\xi, \end{aligned} \quad (4.4)$$

$$\begin{aligned} U_h(q_h)^n &= \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \beta_\tau(e^{-\xi\tau})^{\alpha-2} [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \mu(e^{-\xi\tau}) (f_h(0) + P_h q_h(0)) d\xi \\ &= t_n (f_h(0) + P_h q_h(0)) \\ &\quad + \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \beta_\tau(e^{-\xi\tau})^{-2} [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \mu(e^{-\xi\tau}) \Delta_h P_h (f(0) + q_h(0)) d\xi, \end{aligned} \quad (4.5)$$

respectively, where $\xi^\alpha = (\xi^\alpha - \Delta_h) + \Delta_h$ and $\beta_\tau(e^{-\xi\tau})^\alpha = (\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h) + \Delta_h$ are applied, $\beta_\tau(\cdot)$ is given by (3.18) and $\mu(\cdot)$ is defined by (4.1).

Lemma 4.2. For $f_h(t) = f_h(0)$ and $q_h(t) = q_h(0)$, let $u_h(t_n)$ and $U_h(q_h)^n$ be solutions to (2.22) and (3.31), respectively. Then we have

$$\|u_h(t_n) - U_h(q_h)^n\| \leq C \tau^2 t_n^{\alpha-1} \|\Delta_h P_h (f(0) + q_h(0))\|, \quad (4.6)$$

where the constant C is independent of τ .

Proof. As $|\xi| \geq c\tau^{-1}$ in $\Gamma_{\theta, \kappa} \setminus \Gamma_{\theta, \kappa}^\tau$, we deduce from the estimate $\|(\xi^\alpha - \Delta_h)^{-1}\| \leq C|\xi|^{-\alpha}$ that

$$\left\| \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa} \setminus \Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \xi^{-2} (\xi^\alpha - \Delta_h)^{-1} \Delta_h P_h (f(0) + q_h(0)) d\xi \right\| \leq C \tau^2 t_n^{\alpha-1} \|\Delta_h P_h (f(0) + q_h(0))\|.$$

Then, the estimate (4.6) is derived from (4.4), (4.5) and Lemmas 3.4 and 4.1. \square

For $f_h(t) = t f_h'(0)$ and $q_h(t) = t q_h'(0)$, it also obtains from (2.26) and Theorem 3.2 that the solutions $u_h(t_n)$ and $U_h(q_h)^n$ to (2.22) and (3.31) are in the form of

$$u_h(t_n) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t_n} \xi^{\alpha-3} (\xi^\alpha - \Delta_h)^{-1} (f_h'(0) + P_h q_h'(0)) d\xi, \quad (4.7)$$

$$\begin{aligned} U_h(q_h)^n &= \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_n} \frac{\tau^2 e^{-\xi\tau}}{(1 - e^{-\xi\tau})^2} \beta_\tau(e^{-\xi\tau})^{\alpha-1} \\ &\quad [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \gamma(e^{-\xi\tau}) (f_h'(0) + P_h q_h'(0)) d\xi, \end{aligned} \quad (4.8)$$

where $\beta_\tau(\cdot)$ is given in (3.18) and $\gamma(\cdot)$ is defined by (4.1). Note that the scheme (3.31) for $f_h(t) = t f_h'(0)$ and $q_h(t) = t q_h'(0)$ is identical to the one in [6], and the error estimate has been obtained in [6, Lemma 3.4].

Lemma 4.3 ([6]). For $f_h(t) = t f_h'(0)$ and $q_h(t) = t q_h'(0)$, let $u_h(t_n)$ and $U_h(q_h)^n$ be solutions to (2.22) and (3.31), respectively. Then we have

$$\|u_h(t_n) - U_h(q_h)^n\| \leq C \tau^2 \|f'(0) + q_h'(0)\|, \quad (4.9)$$

where the constant C is independent of τ .

Next, we consider the case of $f_h(t) = (t * f_h'')(t)$ and $q_h(t) = (t * q_h'')(t)$, and state the result in Lemma 4.5. It follows from (2.26) and (2.28) that the solution $u_h(t_n)$ to (2.22) at time t_n with $f_h(t) = (t * f_h'')(t)$ and $q_h(t) = (t * q_h'')(t)$ is given by

$$u_h(t_n) = (E_h * (f + q_h))(t_n) = (E_h * t * (f'' + q_h''))(t_n) = ((E_h * t) * (f'' + q_h''))(t_n), \quad (4.10)$$

with $E_h(t)$ defined in (2.28) and

$$(E_h * t)(t) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t} \xi^{\alpha-3} (\xi^\alpha - \Delta_h)^{-1} P_h d\xi. \quad (4.11)$$

Analogous to the representation of U_h^n in Theorem 3.2, the solution $U_h(q_h)^n$ to (3.31) can be expressed by

$$U_h(q_h)^n = \tau \sum_{j=1}^n E_\tau^{n-j} (f^{j-\frac{1}{2}} + q_h^{j-\frac{1}{2}}), \quad (4.12)$$

where E_τ^n is given in (3.17). Then we obtain

$$\begin{aligned} U_h(q_h)^n &= (\mathcal{E}_\tau * (f + q_h))(t_n) = (\mathcal{E}_\tau * t * (f'' + q_h''))(t_n) \\ &= ((\mathcal{E}_\tau * t) * (f'' + q_h''))(t_n), \end{aligned} \quad (4.13)$$

where

$$\mathcal{E}_\tau(t) = \tau \sum_{j=0}^{\infty} E_\tau^j \delta_{t_{j+\frac{1}{2}}}(t), \quad (4.14)$$

with $\delta_{t_{j+\frac{1}{2}}}(t)$ being the Dirac delta function at $t_{j+\frac{1}{2}}$.

Lemma 4.4. Let $E_h(t)$ and $\mathcal{E}_\tau(t)$ be given by (2.28) and (4.14). Then we have

$$\|((E_h - \mathcal{E}_\tau) * t)(t)\| \leq C\tau^2, \quad \forall t \in (t_{n-1}, t_n], \quad n = 1, 2, \dots, N, \quad (4.15)$$

where the constant C is independent of τ .

Proof. We first prove (4.15) for $t = t_n$. The definition of $\mathcal{E}_\tau(t)$ in (4.14) follows that

$$\begin{aligned} \sum_{n=1}^{\infty} (\mathcal{E}_\tau * t)(t_n) \zeta^n &= \tau \sum_{n=1}^{\infty} \sum_{j=0}^{n-1} (t_n - t_{j+\frac{1}{2}}) E_\tau^j \zeta^n \\ &= \left(\frac{1}{2} + \frac{\zeta}{2}\right) \left(\tau \sum_{n=0}^{\infty} E_\tau^n \zeta^n\right) \left(\sum_{n=0}^{\infty} t_n \zeta^n\right) \\ &= \frac{\tau \zeta}{(1 - \zeta)^2} \beta_\tau(\zeta)^{\alpha-1} [\beta_\tau(\zeta)^\alpha - \Delta_h]^{-1} \gamma(\zeta), \end{aligned}$$

where $\gamma(\cdot)$ is defined by (4.1). By Cauchy's integral formula, we have

$$(\mathcal{E}_\tau * t)(t_n) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi t_n} \frac{\tau^2 e^{-\xi \tau}}{(1 - e^{-\xi \tau})^2} \beta_\tau(e^{-\xi \tau})^{\alpha-1} [\beta_\tau(e^{-\xi \tau})^\alpha - \Delta_h]^{-1} \gamma(e^{-\xi \tau}) d\xi. \quad (4.16)$$

Then it obtains from (4.11), (4.16) and Lemma 4.3 that

$$\|((E_h - \mathcal{E}_\tau) * t)(t_n)\| \leq C\tau^2. \quad (4.17)$$

Next we confirm that (4.15) holds for any $t \in (t_{n-1}, t_n)$. Taking the Taylor expansions of the functions $E_h * t$ and $\mathcal{E}_\tau * t$ at t_n , it follows that

$$(E_h * t)(t) = (E_h * t)(t_n) + (t - t_n)(E_h * 1)(t_n) + \int_{t_n}^t (t - s) E_h(s) ds, \quad (4.18)$$

$$(\mathcal{E}_\tau * t)(t) = (\mathcal{E}_\tau * t)(t_n) + (t - t_n)(\mathcal{E}_\tau * 1)(t_n) + \int_{t_n}^t (t - s)\mathcal{E}_\tau(s)ds. \quad (4.19)$$

It yields from Lemma 4.2 that $\|((E_h - \mathcal{E}_\tau) * 1)(t_n)\| \leq C\tau$. The definition of \mathcal{E}_τ in (4.14) implies that

$$\left\| \int_{t_n}^t (t - s)\mathcal{E}_\tau(s)ds \right\| \leq \tau^2 \|E_\tau^{n-1}\| \leq C\tau^2,$$

together with which and the boundedness of the operator $E_h(\cdot)$ in (2.28) obtains (4.15) for any $t \in (t_{n-1}, t_n)$. \square

Lemma 4.5. For $f_h = (t * f_h'')(t)$, $q_h = (t * q_h'')(t)$, let $u_h(t_n)$ and $U_h(q_h)^n$ be solutions to (2.22) and (3.31), respectively. Then we have

$$\|u_h(t_n) - U_h(q_h)^n\| \leq C\tau^2 \int_0^{t_n} \|f''(s) + q_h''(s)\|ds, \quad (4.20)$$

where the constant C is independent of τ .

Proof. It follows from (4.10) and (4.13) that

$$\|u_h(t_n) - U_h(q_h)^n\| = \|((E_h - \mathcal{E}_\tau) * t * (f'' + q_h''))(t_n)\|,$$

which directly obtains the estimate (4.20) by applying Lemma 4.4. \square

To this end, we are ready to estimate the error $\|\mathbf{u}_h - \mathbf{U}_h(\mathbf{q}_h)\|$ in the following lemma.

Lemma 4.6. Let $u_h(t_n)$ and $U_h(q_h)^n$ be solutions to (2.22) and (3.31), then we have

$$\begin{aligned} \|\mathbf{u}_h - \mathbf{U}_h(\mathbf{q}_h)\| &\leq C\tau^{\min\{\frac{3}{2}+\alpha, 2\}} \|\Delta_h P_h(f(0) + q_h(0))\| \\ &\quad + C\tau^2 [\|f'(0) + q_h'(0)\| + \|f'' + q_h''\|_{L^2(0,T;L^2(\Omega))}], \end{aligned} \quad (4.21)$$

where the constant C is independent of τ .

Proof. It follows from Lemmas 4.2, 4.3 and 4.5 that

$$\begin{aligned} \|u_h(t_n) - U_h(q_h)^n\| &\leq C\tau^2 t_n^{\alpha-1} \|\Delta_h P_h(f(0) + q_h(0))\| + C\tau^2 \|f'(0) + q_h'(0)\| \\ &\quad + C\tau^2 \int_0^{t_n} \|f''(s) + q_h''(s)\|ds \\ &=: I_n + II_n + III_n. \end{aligned} \quad (4.22)$$

On one hand, with the fact $2t_n \geq t_{n+1}$ for $n \geq 1$, we derive that

$$\begin{aligned} \left(\tau \sum_{n=1}^N I_n^2\right)^{\frac{1}{2}} &\leq C\left(\tau \sum_{n=1}^N \tau^4 t_n^{2\alpha-2}\right)^{\frac{1}{2}} \|\Delta_h P_h(f(0) + q_h(0))\| \\ &\leq C\tau^2 \left(\sum_{n=1}^N \int_{t_n}^{t_{n+1}} t^{2\alpha-2} dt\right)^{\frac{1}{2}} \|\Delta_h P_h(f(0) + q_h(0))\| \\ &\leq C\tau^{\min\{\frac{3}{2}+\alpha, 2\}} \|\Delta_h P_h(f(0) + q_h(0))\|. \end{aligned} \quad (4.23)$$

On the other hand, it has

$$\left(\tau \sum_{n=1}^N II_n^2\right)^{\frac{1}{2}} \leq C\left(\tau \sum_{n=1}^N \tau^4\right)^{\frac{1}{2}} \|f'(0) + q_h'(0)\| \leq C\tau^2 \|f'(0) + q_h'(0)\|. \quad (4.24)$$

In addition,

$$\begin{aligned} \left(\tau \sum_{n=1}^N III_n^2\right)^{\frac{1}{2}} &\leq C\left(\tau \sum_{n=1}^N \tau^4 \int_0^{t_n} \|f''(s) + q_h''(s)\|^2 ds\right)^{\frac{1}{2}} \\ &\leq C\tau^2 \|f''(s) + q_h''(s)\|_{L^2(0,T;L^2(\Omega))}. \end{aligned} \quad (4.25)$$

Then the result (4.21) is obtained by (4.23)-(4.25). \square

Remark 4.7. The estimate (4.6) in Lemma 4.2 imposes higher spatial regularity of f and q at the initial time, which is crucial to derive the optimal error estimate (4.21) in Lemma 4.6. Otherwise, it was obtained in [6, Lemma 3.3] that

$$\|u_h(t_n) - U_h(q_h)^n\| \leq C\tau^2 t_n^{-1} \|f_h(0) + q_h(0)\|,$$

then it will result in the following error estimate

$$\begin{aligned} \|u_h - U_h(q_h)\| &\leq C\tau^{\frac{3}{2}} \|f_h(0) + q_h(0)\| \\ &\quad + C\tau^2 [\|f'(0) + q'_h(0)\| + \|f'' + q''_h\|_{L^2(0,T;L^2(\Omega))}], \end{aligned}$$

which is lower than the convergence order $O(\tau^{\min\{\frac{3}{2}+\alpha, 2\}})$ in (4.21). In addition, by using (2.25), (2.27), (2.28), Lemmas 2.5-2.6 and the Sobolev imbedding $H^1(0, T) \hookrightarrow C[0, T]$, we can obtain that $\|\Delta_h P_h q_h(0)\| \leq C$ is satisfied when $U_{ad} = L^2(0, T; L^2(\Omega))$.

4.2 Error estimate of $\|z_h - Z_h(u_h)\|$

In this subsection, we derive the error estimate of $\|z_h - Z_h(u_h)\|$ for the semidiscrete scheme (2.23) and fully discrete scheme (3.33). It is noticed that the temporal error analysis for the discrete adjoint equation (3.33) is largely different from that for the discrete state equation (3.31). Then we first meticulously analyze the error estimate of $\|z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}}\|$ for each term in the Taylor expansions of $u_h(t)$ and $u_d(t)$ at T , that is

$$\begin{aligned} u_h(t) &= u_h(T) - (T-t)u'_h(T) + \int_t^T (s-t)u''_h(s)ds, \\ u_d(t) &= u_d(T) - (T-t)u'_d(T) + \int_t^T (s-t)u''_d(s)ds. \end{aligned}$$

For the case of $u_h(t) = u_h(T)$ and $u_d(t) = u_d(T)$, together with the splittings $\xi^\alpha = (\xi^\alpha - \Delta_h) + \Delta_h$ and $\beta_\tau(e^{-\xi\tau})^\alpha = (\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h) + \Delta_h$, it implies from (2.27) and (2.28) that the semidiscrete solution $z_h(t_{n-\frac{1}{2}})$ to (2.23) can also be represented by

$$\begin{aligned} z_h(t_{n-\frac{1}{2}}) &= \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi(T-t_{n-\frac{1}{2}})} \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} P_h(u_h(T) - u_d(T)) d\xi \\ &= (T-t_{n-\frac{1}{2}}) P_h(u_h(T) - u_d(T)) \\ &\quad + \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi(T-t_{n-\frac{1}{2}})} \xi^{-2} (\xi^\alpha - \Delta_h)^{-1} \Delta_h P_h(u_h(T) - u_d(T)) d\xi, \end{aligned} \tag{4.26}$$

and the fully discrete solution $Z_h(u_h)^{n-\frac{1}{2}}$ to (3.33) can be obtained from (3.16) in Theorem 3.2 as follows

$$\begin{aligned} Z_h(u_h)^{n-\frac{1}{2}} &= (T-t_{n-\frac{1}{2}}) P_h(u_h(T) - u_d(T)) \\ &\quad + \frac{1}{4\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi(T-t_{n-1})} \beta_\tau(e^{-\xi\tau})^{-2} [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \mu(e^{-\xi\tau}) \Delta_h P_h(u_h(T) - u_d(T)) d\xi \\ &\quad + \frac{1}{4\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi(T-t_n)} \beta_\tau(e^{-\xi\tau})^{-2} [\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \mu(e^{-\xi\tau}) \Delta_h P_h(u_h(T) - u_d(T)) d\xi, \end{aligned} \tag{4.27}$$

where $\beta_\tau(e^{-\xi\tau})$ and $\mu(e^{-\xi\tau})$ are given by (3.18) and (4.1), respectively.

Lemma 4.8. For $u_h(t) = u_h(T)$ and $u_d(t) = u_d(T)$, let $z_h(t_{n-\frac{1}{2}})$ and $Z_h(u_h)^{n-\frac{1}{2}}$ be solutions to (2.23) and (3.33) given by (4.26) and (4.27), respectively. Then we have

$$\|z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}}\| \leq C\tau^2(T - t_{n-\frac{1}{2}})^{\alpha-1}[\|\Delta_h u_h(T)\| + \|\Delta u_d(T)\|], \quad (4.28)$$

where the constant C is independent of τ .

Proof. From (4.26) and (4.27), it obtains that

$$\begin{aligned} & z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}} \\ &= \frac{1}{4\pi i} \int_{\Gamma_{\theta,\kappa} \setminus \Gamma_{\theta,\kappa}^\tau} e^{\xi(T-t_{n-\frac{1}{2}})} \mathcal{M}(\xi) \Delta_h P_h(u_h(T) - u_d(T)) d\xi \\ &+ \frac{1}{4\pi i} \int_{\Gamma_{\theta,\kappa}^\tau} e^{\xi(T-t_{n-\frac{1}{2}})} \mathcal{N}(\xi) \Delta_h P_h(u_h(T) - u_d(T)) d\xi, \end{aligned} \quad (4.29)$$

where $\mathcal{M}(\xi)$ and $\mathcal{N}(\xi)$ are given by

$$\begin{aligned} \mathcal{M}(\xi) &:= 2\xi^{-2}(\xi^\alpha - \Delta_h)^{-1}, \\ \mathcal{N}(\xi) &:= 2\xi^{-2}(\xi^\alpha - \Delta_h)^{-1} - (e^{-\frac{\xi\tau}{2}} + e^{\frac{\xi\tau}{2}})\beta_\tau(e^{-\xi\tau})^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\mu(e^{-\xi\tau}). \end{aligned}$$

It derives from Lemmas 2.5, 3.4 and 4.1 the following two estimates

$$\|\mathcal{M}(\xi)\| \leq C|\xi|^{-\alpha-2} \leq C\tau^2|\xi|^{-\alpha}, \quad \forall \xi \in \Gamma_{\theta,\kappa} \setminus \Gamma_{\theta,\kappa}^\tau \quad (4.30)$$

and

$$\begin{aligned} \|\mathcal{N}(\xi)\| &\leq \|2\xi^{-2}(\xi^\alpha - \Delta_h)^{-1} - 2\xi^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \\ &+ 2\xi^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} - 2\beta_\tau(e^{-\xi\tau})^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \\ &+ 2\beta_\tau(e^{-\xi\tau})^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} - 2\beta_\tau(e^{-\xi\tau})^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\mu(e^{-\xi\tau}) \\ &+ 2\beta_\tau(e^{-\xi\tau})^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\mu(e^{-\xi\tau}) \\ &- (e^{-\frac{\xi\tau}{2}} + e^{\frac{\xi\tau}{2}})\beta_\tau(e^{-\xi\tau})^{-2}[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\mu(e^{-\xi\tau})\| \\ &\leq C\tau^2|\xi|^{-\alpha}, \quad \forall \xi \in \Gamma_{\theta,\kappa}^\tau, \end{aligned} \quad (4.31)$$

where the inequality $|2 - e^{-\frac{1}{2}\xi\tau} - e^{\frac{1}{2}\xi\tau}| \leq C\tau^2|\xi|^2$ is employed. Then the estimate (4.28) is obtained from (4.29), (4.30), (4.31) and the inequality $\|\Delta_h P_h v\| \leq C\|\Delta v\|$ for any $v \in \dot{H}^2(\Omega)$ in [3, (2.13)]. \square

The term $\|\Delta_h u_h(T)\|$ in (4.28) is actually bounded by using (2.26), (2.28), Lemmas 2.5-2.6 and the Sobolev imbedding $H^1(0, T) \hookrightarrow C[0, T]$.

Next we consider the error estimate for the case of $u_h(t) = (T-t)u'_h(T)$ and $u_d(t) = (T-t)u'_d(T)$, and obtain the result in Lemma 4.9. Similarly by (2.27) and (3.16), the seimidiscrete solution $z_h(t_{n-\frac{1}{2}})$ to (2.23) and the fully discrete solution $Z_h(u_h)^{n-\frac{1}{2}}$ to (3.33) with $u_h(t) = (T-t)u'_h(T)$ and $u_d(t) = (T-t)u'_d(T)$ can be represented by

$$z_h(t_{n-\frac{1}{2}}) = \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}} e^{\xi(T-t_{n-\frac{1}{2}})} \xi^{\alpha-3}(\xi^\alpha - \Delta_h)^{-1} P_h(u'_h(T) - u'_d(T)) d\xi, \quad (4.32)$$

$$\begin{aligned} Z_h(u_h)^{n-\frac{1}{2}} &= \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}^\tau} e^{\xi(T-t_n)} \frac{\tau^2 e^{-\xi\tau}}{(1 - e^{-\xi\tau})^2} \beta_\tau(e^{-\xi\tau})^\alpha \\ &[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi\tau})^{-1} P_h(u'_h(T) - u'_d(T)) d\xi, \end{aligned} \quad (4.33)$$

respectively, where $\delta_\tau(\cdot)$ and $\beta_\tau(\cdot)$ are defined in (3.18).

Lemma 4.9. For $u_h(t) = (T - t)u'_h(T)$ and $u_d(t) = (T - t)u'_d(T)$, let $z_h(t_{n-\frac{1}{2}})$ and $Z_h(u_h)^{n-\frac{1}{2}}$ be solutions to (2.23) and (3.33) given by (4.32) and (4.33), respectively. Then we have the estimate

$$\|z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}}\| \leq C\tau^2 \|u'_h(T) - u'_d(T)\|, \quad (4.34)$$

where the constant C is independent of τ .

Proof. Let $\mathcal{C}(\xi)$ and $\mathcal{F}(\xi)$ be defined by

$$\mathcal{C}(\xi) := \xi^{\alpha-3}(\xi^\alpha - \Delta_h)^{-1}P_h,$$

$$\mathcal{F}(\xi) := e^{\frac{\xi\tau}{2}}\xi^{\alpha-3}(\xi^\alpha - \Delta_h)^{-1}P_h - \frac{\tau^2 e^{-\xi\tau}}{(1 - e^{-\xi\tau})^2}\beta_\tau(e^{-\xi\tau})^\alpha[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\delta_\tau(e^{-\xi\tau})^{-1}P_h.$$

From Lemmas 2.5, 3.3 and 3.4, it obtains that $\|\mathcal{C}(\xi)\| \leq C|\xi|^{-3}$ and

$$\begin{aligned} \|\mathcal{F}(\xi)\| &\leq \|e^{\frac{\xi\tau}{2}}\xi^{\alpha-3}(\xi^\alpha - \Delta_h)^{-1} - \xi^{\alpha-2}(\xi^\alpha - \Delta_h)^{-1}\delta_\tau(e^{-\xi\tau})^{-1} \\ &\quad + \xi^{\alpha-2}(\xi^\alpha - \Delta_h)^{-1}\delta_\tau(e^{-\xi\tau})^{-1} \\ &\quad - \frac{\tau^2 e^{-\xi\tau}}{(1 - e^{-\xi\tau})^2}\beta_\tau(e^{-\xi\tau})^\alpha[\beta_\tau(e^{-\xi\tau})^\alpha - \Delta_h]^{-1}\delta_\tau(e^{-\xi\tau})^{-1}\| \\ &\leq C\tau^2|\xi|^{-1}, \quad \forall \xi \in \Gamma_{\theta,\kappa}^\tau, \end{aligned} \quad (4.35)$$

where the estimate $|\xi^{-1}e^{\frac{1}{2}\xi\tau} - \delta_\tau(e^{-\xi\tau})^{-1}| \leq C\tau^2|\xi|$ is applied.

Then we derive from (4.32) and (4.33) that

$$\begin{aligned} \|z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}}\| &\leq \left\| \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa} \setminus \Gamma_{\theta,\kappa}^\tau} e^{\xi(T-t_{n-\frac{1}{2}})} \mathcal{C}(\xi) d\xi \right\| \|u'_h(T) - u'_d(T)\| \\ &\quad + \left\| \frac{1}{2\pi i} \int_{\Gamma_{\theta,\kappa}^\tau} e^{\xi(T-t_n)} \mathcal{F}(\xi) d\xi \right\| \|u'_h(T) - u'_d(T)\| \\ &\leq C\tau^2 \|u'_h(T) - u'_d(T)\|, \end{aligned}$$

which completes the proof. \square

In the following, we consider the terms $u_h(t) = \int_t^T (s - t)u''_h(s)ds$ and $u_d(t) = \int_t^T (s - t)u''_d(s)ds$, which yields that $u_h(T) = 0$ and $u_d(T) = 0$. Then we obtain from (2.27) that the corresponding semidiscrete solution $z_h(t_{n-\frac{1}{2}})$ to (2.23) is as follows

$$\begin{aligned} z_h(t_{n-\frac{1}{2}}) &= \int_{t_{n-\frac{1}{2}}}^T E_h(s - t_{n-\frac{1}{2}}) \int_s^T (r - s)(u''_h(r) - u''_d(r))drds \\ &= \int_{t_{n-\frac{1}{2}}}^T \int_{t_{n-\frac{1}{2}}}^r E_h(s - t_{n-\frac{1}{2}})(r - s)(u''_h(r) - u''_d(r))dsdr \\ &= \int_{t_{n-\frac{1}{2}}}^T (E_h * t)(r - t_{n-\frac{1}{2}})(u''_h(r) - u''_d(r))dr. \end{aligned} \quad (4.36)$$

It also derives from (3.16) that the fully discrete solution $Z_h(u_h)^{n-\frac{1}{2}}$ to (3.33) is represented accordingly by

$$Z_h(u_h)^{n-\frac{1}{2}} = \tau \sum_{j=0}^{N-n} E_\tau^{N-n-j}(u_h^{N-j} - u_d^{N-j}). \quad (4.37)$$

Let $\delta_{t_j}(t)$ be the Dirac delta function at t_j and

$$\mathcal{H}_\tau(t) := \tau \sum_{j=0}^{\infty} E_\tau^j \delta_{t_j}(t), \quad (4.38)$$

then we further have

$$\begin{aligned} Z_h(u_h)^{n-\frac{1}{2}} &= \int_{t_n}^T \mathcal{H}_\tau(s - t_n)(u_h(s) - u_d(s)) ds \\ &= \int_{t_n}^T \mathcal{H}_\tau(s - t_n) \int_s^T (r - s)(u_h''(r) - u_d''(r)) dr ds \\ &= \int_{t_n}^T \int_{t_n}^r \mathcal{H}_\tau(s - t_n)(r - s)(u_h''(r) - u_d''(r)) ds dr \\ &= \int_{t_n}^T (\mathcal{H}_\tau * t)(r - t_n)(u_h''(r) - u_d''(r)) dr. \end{aligned} \quad (4.39)$$

Lemma 4.10. Let $E_h(t)$ and $\mathcal{H}_\tau(t)$ be defined by (2.28) and (4.38), respectively. Then we have

$$\|(E_h * t)(t + \frac{\tau}{2}) - (\mathcal{H}_\tau * t)(t)\| \leq C\tau^2, \quad (4.40)$$

where $t \in [0, T - \tau]$, and the constant C is independent of τ .

Proof. For any $t \in [t_m, t_{m+1})$ with $0 \leq m \leq N - n - 1$ and $n = 1, 2, \dots, N$, we take the Taylor expansions of operators $(E_h * t)(t + \frac{\tau}{2})$ and $(\mathcal{H}_\tau * t)(t)$ at time t_m and get

$$\begin{aligned} (E_h * t)(t + \frac{\tau}{2}) &= (E_h * t)(t_m + \frac{\tau}{2}) + (t - t_m)(E_h * 1)(t_m + \frac{\tau}{2}) \\ &\quad + \int_{t_m + \frac{\tau}{2}}^{t + \frac{\tau}{2}} (t + \frac{\tau}{2} - s) E_h(s) ds, \end{aligned} \quad (4.41)$$

$$(\mathcal{H}_\tau * t)(t) = (\mathcal{H}_\tau * t)(t_m) + (t - t_m)(\mathcal{H}_\tau * 1)(t_m) + \int_{t_m}^t (t - s) \mathcal{H}_\tau(s) ds. \quad (4.42)$$

It follows from (4.11) that

$$(E_h * t)(t_m + \frac{\tau}{2}) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}} e^{\xi(t_m + \frac{\tau}{2})} \xi^{\alpha-3} (\xi^\alpha - \Delta_h)^{-1} d\xi. \quad (4.43)$$

By the definition of the operator $\mathcal{H}_\tau(t)$ in (4.38), it implies that

$$(\mathcal{H}_\tau * t)(t_m) = \tau \sum_{j=0}^m E_\tau^j(t_m - t_j), \quad (4.44)$$

then we further derive from (3.17) that

$$\begin{aligned} \sum_{m=0}^{\infty} (\mathcal{H}_\tau * t)(t_m) \zeta^m &= \tau \sum_{m=0}^{\infty} \sum_{j=0}^m E_\tau^j(t_m - t_j) \zeta^m \\ &= \left(\tau \sum_{m=0}^{\infty} E_\tau^m \zeta^m \right) \left(\sum_{m=0}^{\infty} t_m \zeta^m \right) \\ &= \beta_\tau(\zeta)^\alpha [\beta_\tau(\zeta)^\alpha - \Delta_h]^{-1} \delta_\tau(\zeta)^{-1} \frac{\tau \zeta}{(1 - \zeta)^2}. \end{aligned} \quad (4.45)$$

From (4.45) and Cauchy's integral formula, it obtains that

$$(\mathcal{H}_\tau * t)(t_m) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_m} \frac{\tau^2 e^{-\xi \tau}}{(1 - e^{-\xi \tau})^2} \beta_\tau(e^{-\xi \tau})^\alpha [\beta_\tau(e^{-\xi \tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi \tau})^{-1} d\xi. \quad (4.46)$$

Then by the similar approach as in the proof of Lemma 4.9, we have

$$\|(E_h * t)(t_m + \frac{\tau}{2}) - (\mathcal{H}_\tau * t)(t_m)\| \leq C\tau^2. \quad (4.47)$$

Next we consider to analyze the following estimate

$$\|(E_h * 1)(t_m + \frac{\tau}{2}) - (\mathcal{H}_\tau * 1)(t_m)\| \leq C\tau. \quad (4.48)$$

From the definition of $E_h(\cdot)$ in (2.28), we have

$$(E_h * 1)(t_m + \frac{\tau}{2}) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi(t_m + \frac{\tau}{2})} \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} d\xi. \quad (4.49)$$

By the similar approach for deriving (4.44), it obtains

$$(\mathcal{H}_\tau * 1)(t_m) = \frac{1}{2\pi i} \int_{\Gamma_{\theta, \kappa}^\tau} e^{\xi t_m} \frac{\tau}{1 - e^{-\xi \tau}} \beta_\tau(e^{-\xi \tau})^\alpha [\beta_\tau(e^{-\xi \tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi \tau})^{-1} d\xi. \quad (4.50)$$

With Lemmas 2.5, 3.3 and 3.4, it also holds that

$$\begin{aligned} & \left\| e^{\frac{\xi \tau}{2}} \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} - \frac{\tau}{1 - e^{-\xi \tau}} \beta_\tau(e^{-\xi \tau})^\alpha [\beta_\tau(e^{-\xi \tau})^\alpha - \Delta_h]^{-1} \delta_\tau(e^{-\xi \tau})^{-1} \right\| \\ & \leq \left\| e^{\frac{\xi \tau}{2}} \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} - \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} \right\| \\ & \quad + \left\| \xi^{\alpha-2} (\xi^\alpha - \Delta_h)^{-1} - \delta_\tau(e^{-\xi \tau})^{-2} \xi^\alpha (\xi^\alpha - \Delta_h)^{-1} \right\| \\ & \quad + \left\| \delta_\tau(e^{-\xi \tau})^{-2} \xi^\alpha (\xi^\alpha - \Delta_h)^{-1} - \delta_\tau(e^{-\xi \tau})^{-2} \beta_\tau(e^{-\xi \tau})^\alpha [\beta_\tau(e^{-\xi \tau})^\alpha - \Delta_h]^{-1} \right\| \\ & \leq C\tau |\xi|^{-1} + C\tau^2, \quad \forall \xi \in \Gamma_{\theta, \kappa}^\tau, \end{aligned}$$

then (4.48) is derived, which further implies that

$$(t - t_m) \|(E_h * 1)(t_m + \frac{\tau}{2}) - (\mathcal{H}_\tau * 1)(t_m)\| \leq C\tau^2. \quad (4.51)$$

Due to $\|E_h(t)\| \leq C$ and $\|E_\tau^m\| \leq C$, we derive the following estimates

$$\left\| \int_{t_m + \frac{\tau}{2}}^{t + \frac{\tau}{2}} (t + \frac{\tau}{2} - s) E_h(s) ds \right\| \leq C\tau^2, \quad (4.52)$$

and

$$\left\| \int_{t_m}^t (t - s) \mathcal{H}_\tau(s) ds \right\| \leq \tau^2 \|E_\tau^m\| \leq C\tau^2. \quad (4.53)$$

Therefore, the result (4.40) is obtained from (4.47), (4.51), (4.52) and (4.53). \square

Lemma 4.11. For $u_h(t) = \int_t^T (s - t) u_h''(s) ds$ and $u_d(t) = \int_t^T (s - t) u_d''(s) ds$, let $z_h(t_{n-\frac{1}{2}})$ and $Z_h(u_h)^{n-\frac{1}{2}}$ be solutions to (2.23) and (3.33). Then we obtain the estimate

$$\|z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}}\| \leq C\tau^2 \int_{t_{n-\frac{1}{2}}}^T \|u_h''(s) - u_d''(s)\| ds, \quad (4.54)$$

where the constant C is independent of τ .

Proof. The formulae (4.36) and (4.39) imply that

$$\begin{aligned}
& \|z_h(t_{n-\frac{1}{2}}) - Z_h(u_h)^{n-\frac{1}{2}}\| \\
& \leq \int_{t_{n-\frac{1}{2}}}^{t_n} \|(E_h * t)(r - t_{n-\frac{1}{2}})\| \|u_h''(r) - u_d''(r)\| dr \\
& \quad + \int_{t_n}^T \|(E_h * t)(r - t_{n-\frac{1}{2}}) - (\mathcal{H}_\tau * t)(r - t_n)\| \|u_h''(r) - u_d''(r)\| dr \\
& =: IV + V.
\end{aligned}$$

For the term IV , it yields from (4.11) and Lemma 2.5 that

$$IV \leq C\tau^2 \int_{t_{n-\frac{1}{2}}}^{t_n} \|u_h''(r) - u_d''(r)\| dr.$$

By (4.40) in Lemma 4.10, we obtain the estimate for the term V as follows

$$V \leq C\tau^2 \int_{t_n}^T \|u_h''(r) - u_d''(r)\| dr.$$

Thus the result (4.54) is derived by combining the above two estimates. \square

By the results in Lemmas 4.8, 4.9 and 4.11, it directly implies that

$$\begin{aligned}
\|Z_h(u_h)^{n-\frac{1}{2}} - z_h(t_{n-\frac{1}{2}})\| & \leq C\tau^2(T - t_{n-\frac{1}{2}})^{\alpha-1} [\|\Delta_h u_h(T)\| + \|\Delta u_d(T)\|] \\
& \quad + C\tau^2 \|u_h'(T) - u_d'(T)\| + C\tau^2 \int_{t_{n-\frac{1}{2}}}^T \|u_h''(s) - u_d''(s)\| ds,
\end{aligned} \tag{4.55}$$

where the constant C is independent of τ , $z_h(t_{n-\frac{1}{2}})$ and $Z_h(u_h)^{n-\frac{1}{2}}$ are solutions to (2.23) and (3.33), respectively. Therefore, by the similar approach as in the proof of Lemma 4.6, we can obtain the error estimate $\|z_h - Z_h(u_h)\|$ in Lemma 4.12.

Lemma 4.12. *Let z_h and $Z_h(u_h)^{n-\frac{1}{2}}$ be solutions to (2.23) and (3.33), respectively, then we have the following estimate*

$$\begin{aligned}
\|z_h - Z_h(u_h)\| & \leq C\tau^{\min\{\frac{3}{2}+\alpha, 2\}} [\|\Delta_h u_h(T)\| + \|\Delta u_d(T)\|] \\
& \quad + C\tau^2 [\|u_h'(T) - u_d'(T)\| + \|u_h''(s) - u_d''(s)\|_{L^2(0,T;L^2(\Omega))}],
\end{aligned} \tag{4.56}$$

where the constant C is independent of τ .

4.3 Fully discrete error estimates

With the results obtained at hand in Sections 4.1 and 4.2, we are ready to analyze the error estimates of $\|u_h - U_h\|$, $\|z_h - Z_h\|$ and $\|q_h - Q_h\|$ for the fully discrete Crank-Nicolson scheme (3.5)-(3.6) and the semidiscrete scheme (2.20)-(2.21).

Lemma 4.13. *Let u_h and U_h^n be solutions to (2.22) and (3.10), respectively. Then we have*

$$\begin{aligned}
\|u_h - U_h\| & \leq C\|q_h - Q_h\| + C\tau^{\min\{\frac{3}{2}+\alpha, 2\}} \|\Delta_h P_h(f(0) + q_h(0))\| \\
& \quad + C\tau^2 [\|f'(0) + q_h'(0)\| + \|f'' + q_h''\|_{L^2(0,T;L^2(\Omega))}],
\end{aligned} \tag{4.57}$$

where the constant C is independent of τ .

Proof. By the estimate (3.34) in Theorem 3.5 and the triangular inequality, we derive that

$$\begin{aligned} |||\mathbf{u}_h - \mathbf{U}_h||| &\leq |||\mathbf{u}_h - \mathbf{U}_h(\mathbf{q}_h)||| + |||\mathbf{U}_h(\mathbf{q}_h) - \mathbf{U}_h||| \\ &\leq |||\mathbf{u}_h - \mathbf{U}_h(\mathbf{q}_h)||| + C|||\mathbf{q}_h - \mathbf{Q}_h|||, \end{aligned}$$

which directly obtains the result (4.57) from Lemma 4.6. \square

The error analysis of $|||\mathbf{q}_h - \mathbf{Q}_h|||$ is derived in the following lemma.

Lemma 4.14. *Let q_h and $Q_h^{n-\frac{1}{2}}$ be solutions to (2.24) and (3.12), respectively, then we have*

$$\begin{aligned} |||\mathbf{q}_h - \mathbf{Q}_h||| &\leq C\tau^{\min\{\frac{3}{2}+\alpha, 2\}} [\|\Delta_h P_h(f(0) + q_h(0))\| + \|\Delta_h u_h(T)\| + \|\Delta u_d(T)\|] \\ &\quad + C\tau^2 [\|f'(0) + q'_h(0)\| + \|u'_h(T) - u'_d(T)\|] \\ &\quad + C\tau^2 [\|f'' + q''_h\|_{L^2(0,T;L^2(\Omega))} + \|u''_h - u''_d\|_{L^2(0,T;L^2(\Omega))}], \end{aligned} \quad (4.58)$$

where the constant C is independent of τ .

Proof. It obtains from (2.25) that $q_h(t_{n-\frac{1}{2}}) = P_{U_{ad}}(-\frac{1}{\gamma}z_h(t_{n-\frac{1}{2}}))$, and then

$$(\gamma q_h(\cdot, t_{n-\frac{1}{2}}) + z_h(\cdot, t_{n-\frac{1}{2}}), v_h - q_h(\cdot, t_{n-\frac{1}{2}})) \geq 0, \quad \forall v_h \in U_{ad}. \quad (4.59)$$

Together with (3.12) and (4.59), it implies that

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

By (3.10)-(3.11), (3.31)-(3.32), and (3.7)-(3.9), we can derive that

$$[\mathbf{q}_h - \mathbf{Q}_h, \mathbf{Z}_h - \mathbf{Z}_h(\mathbf{U}_h(\mathbf{q}_h))] = -|||\mathbf{U}_h(\mathbf{q}_h) - \mathbf{U}_h|||^2 \leq 0.$$

Furthermore, it has from the above estimates and (3.35) in Theorem 3.5 that

$$\begin{aligned} |||\mathbf{q}_h - \mathbf{Q}_h||| &\leq C|||\mathbf{Z}_h(\mathbf{U}_h(\mathbf{q}_h)) - \mathbf{z}_h||| \\ &\leq C|||\mathbf{Z}_h(\mathbf{U}_h(\mathbf{q}_h)) - \mathbf{Z}_h(\mathbf{u}_h)||| + C|||\mathbf{Z}_h(\mathbf{u}_h) - \mathbf{z}_h||| \\ &\leq C|||\mathbf{U}_h(\mathbf{q}_h) - \mathbf{u}_h||| + C|||\mathbf{Z}_h(\mathbf{u}_h) - \mathbf{z}_h|||, \end{aligned} \quad (4.60)$$

from which it obtains the result (4.58) directly from the estimates (4.21) and (4.56). \square

By using (3.36) in Theorem 3.5, we have that

$$\begin{aligned} |||\mathbf{z}_h - \mathbf{Z}_h||| &\leq |||\mathbf{z}_h - \mathbf{Z}_h(\mathbf{u}_h)||| + |||\mathbf{Z}_h(\mathbf{u}_h) - \mathbf{Z}_h||| \\ &\leq |||\mathbf{z}_h - \mathbf{Z}_h(\mathbf{u}_h)||| + C|||\mathbf{u}_h - \mathbf{U}_h|||. \end{aligned} \quad (4.61)$$

Together with (4.61), Lemmas 4.12, 4.13 and 4.14, we finally derive the main result in the following theorem.

Theorem 4.15. *Let (u_h, z_h, q_h) and $(U_h^n, Z_h^{n-\frac{1}{2}}, Q_h^{n-\frac{1}{2}})$ be solutions to the systems (2.22)-(2.24) and (3.10)-(3.12), respectively. If the conditions in Theorem 2.3 are satisfied and the admissible set $U_{ad} = L^2(0, T; L^2(\Omega))$, then we have*

$$\begin{aligned} &|||\mathbf{u}_h - \mathbf{U}_h||| + |||\mathbf{z}_h - \mathbf{Z}_h||| + |||\mathbf{q}_h - \mathbf{Q}_h||| \\ &\leq C\tau^{\min\{\frac{3}{2}+\alpha, 2\}} [\|\Delta_h P_h(f(0) + q_h(0))\| + \|\Delta_h u_h(T)\| + \|\Delta u_d(T)\|] \\ &\quad + C\tau^2 [\|f'(0) + q'_h(0)\| + \|u'_h(T) - u'_d(T)\|] \\ &\quad + C\tau^2 [\|f'' + q''_h\|_{L^2(0,T;L^2(\Omega))} + \|u''_h - u''_d\|_{L^2(0,T;L^2(\Omega))}], \end{aligned}$$

where the constant C is independent of τ .

Remark 4.16. *For the optimal control problem with the box constraint (1.3), the best temporal regularity of q_h is restricted to $W^{1,\infty}$ by the property of the projection operator $P_{U_{ad}}(\cdot)$ in (2.7), see [9, (3.5)] and [40, Corollary 2.1.8]. Then it appears challenging to establish the optimal temporal error estimate for the fully discrete Crank-Nicolson scheme (3.5)-(3.6).*

5 Numerical results

In this section, we present some numerical examples to verify the theoretical convergence result in Theorem 4.15 of the proposed fully discrete Crank-Nicolson scheme (3.5)-(3.6) for solving the optimal control problem (1.1)-(1.2).

Two numerical examples with the admissible set $U_{ad} = L^2(0, T; L^2(\Omega))$ are presented to illustrate the efficiency of the proposed discrete Crank-Nicolson scheme (3.5)-(3.6). We solve the fully discrete system (3.5)-(3.6) by the conjugate gradient method with a stopping tolerance 10^{-8} measuring the gradient of the objective function with respect to \mathbf{Q}_h in (3.5).

Example 5.1. Let $\Omega = (0, 1)$ and $T = 1$. We take $\gamma = 1$ in the optimal control problem (1.1)-(1.2) and set the exact solutions as

$$\begin{aligned} u(x, t) &= t^{1.5+\alpha/4}x(1-x), \\ z(x, t) &= (1-t)^{1.5+\alpha/4}x(1-x), \\ q(x, t) &= -z(x, t). \end{aligned}$$

By simple calculations, it obtains the expressions of f and u_d from (2.3) and (2.4).

To demonstrate the temporal convergence rate of the fully discrete Crank-Nicolson scheme (3.5)-(3.6), we solve the one dimensional optimal control problem in Example 5.1 for $\alpha = 0.1, 0.3, 0.5, 0.7$ and 0.9 with the time step and finite element mesh size $\tau = h = 2^{-k}$, $k = 3, 4, 5, 6$. In Table 1, the errors $\|\mathbf{u}_h - \mathbf{U}_h\|$, $\|\mathbf{z}_h - \mathbf{Z}_h\|$, $\|\mathbf{q}_h - \mathbf{Q}_h\|$ and their temporal convergence rates are reported. It shows that the numerical scheme has the convergence order of $O(\tau^{\min\{\frac{3}{2}+\alpha, 2\}})$ in time, which is consistent with the theoretical convergence order in Theorem 4.15.

Table 1: Errors $\|\mathbf{u}_h - \mathbf{U}_h\|$, $\|\mathbf{z}_h - \mathbf{Z}_h\|$, $\|\mathbf{q}_h - \mathbf{Q}_h\|$ and their temporal convergence rates for Example 5.1.

α	Error	$\tau = 2^{-3}$	$\tau = 2^{-4}$	$\tau = 2^{-5}$	$\tau = 2^{-6}$	Rate
0.10	$\ \mathbf{u}_h - \mathbf{U}_h\ $	6.5791E-04	2.1063E-04	6.8409E-05	2.2409E-05	1.63 (1.6)
	$\ \mathbf{z}_h - \mathbf{Z}_h\ $	1.9146E-03	6.1414E-04	1.9661E-04	6.3162E-05	1.64 (1.6)
	$\ \mathbf{q}_h - \mathbf{Q}_h\ $	1.9147E-03	6.1414E-04	1.9661E-04	6.3162E-05	1.64 (1.6)
0.30	$\ \mathbf{u}_h - \mathbf{U}_h\ $	2.8456E-04	7.8631E-05	2.2295E-05	6.4935E-06	1.82 (1.8)
	$\ \mathbf{z}_h - \mathbf{Z}_h\ $	1.2315E-03	3.4528E-04	9.6767E-05	2.7325E-05	1.83 (1.8)
	$\ \mathbf{q}_h - \mathbf{Q}_h\ $	1.2315E-03	3.4528E-04	9.6767E-05	2.7325E-05	1.83 (1.8)
0.50	$\ \mathbf{u}_h - \mathbf{U}_h\ $	2.1904E-04	5.4259E-05	1.2990E-05	3.0365E-06	2.06 (2.0)
	$\ \mathbf{z}_h - \mathbf{Z}_h\ $	9.7469E-04	2.5903E-04	6.9232E-05	1.8769E-05	1.90 (2.0)
	$\ \mathbf{q}_h - \mathbf{Q}_h\ $	9.7469E-04	2.5903E-04	6.9232E-05	1.8769E-05	1.90 (2.0)
0.70	$\ \mathbf{u}_h - \mathbf{U}_h\ $	2.6789E-04	6.4009E-05	1.4957E-05	3.4005E-06	2.10 (2.0)
	$\ \mathbf{z}_h - \mathbf{Z}_h\ $	8.6773E-04	2.2799E-04	6.0457E-05	1.6277E-05	1.91 (2.0)
	$\ \mathbf{q}_h - \mathbf{Q}_h\ $	8.6773E-04	2.2799E-04	6.0457E-05	1.6277E-05	1.91 (2.0)
0.90	$\ \mathbf{u}_h - \mathbf{U}_h\ $	2.5752E-04	6.0488E-05	1.4254E-05	3.3384E-06	2.09 (2.0)
	$\ \mathbf{z}_h - \mathbf{Z}_h\ $	8.0626E-04	2.1123E-04	5.5724E-05	1.4866E-05	1.92 (2.0)
	$\ \mathbf{q}_h - \mathbf{Q}_h\ $	8.0626E-04	2.1123E-04	5.5724E-05	1.4866E-05	1.92 (2.0)

Example 5.2. Consider the two dimensional optimal control problem (1.1)-(1.2) with $\Omega = (0, 1) \times (0, 1)$, $T = 1$ and $\gamma = 1$. For any $x = (x_1, x_2) \in \Omega$, the exact solution is chosen as

$$u(x, t) = t^{1.5+\alpha/6} \sin(\pi x_1) \sin(\pi x_2),$$

$$z(x, t) = (1 - t)^{1.5+\alpha/6} \sin(\pi x_1) \sin(\pi x_2),$$

$$q(x, t) = -z(x, t),$$

and f and u_d are calculated from (2.3) and (2.4).

We consider the fully discrete Crank-Nicolson scheme (3.5)-(3.6) to solve the two dimensional optimal control problem in Example 5.2. In order to verify its convergence order in time, we choose $\alpha = 0.1, 0.3, 0.5, 0.7, 0.9$, and perform numerical experiments with time step $\tau = 2^{-k}$ ($k = 3, 4, 5, 6, 7$) and finite element mesh size $h = 2^{-9}$. The errors $\|u_h - U_h\|$, $\|z_h - Z_h\|$, $\|q_h - Q_h\|$ and their temporal convergence rates are presented in Table 2, where similar observations as those in Example 5.1 are shown. The scheme also converges by the order of $O(\tau^{\min\{\frac{3}{2}+\alpha, 2\}})$ in time, which confirms the theoretical result in Theorem 4.15.

Table 2: Errors $\|u_h - U_h\|$, $\|z_h - Z_h\|$, $\|q_h - Q_h\|$ and their temporal convergence rates for Example 5.2.

α	Error	$\tau = 2^{-3}$	$\tau = 2^{-4}$	$\tau = 2^{-5}$	$\tau = 2^{-6}$	Rate
0.10	$\ u_h - U_h\ $	1.1646E-03	4.1573E-04	1.4586E-04	5.0255E-05	1.51 (1.6)
	$\ z_h - Z_h\ $	5.4275E-03	1.7262E-03	5.5277E-04	1.7868E-04	1.64 (1.6)
	$\ q_h - Q_h\ $	5.4275E-03	1.7262E-03	5.5277E-04	1.7868E-04	1.64 (1.6)
0.30	$\ u_h - U_h\ $	2.8509E-04	7.6380E-05	2.2607E-05	7.1627E-06	1.77 (1.8)
	$\ z_h - Z_h\ $	3.5268E-03	9.7637E-04	2.7212E-04	7.6976E-05	1.84 (1.8)
	$\ q_h - Q_h\ $	3.5268E-03	9.7637E-04	2.7212E-04	7.6977E-05	1.84 (1.8)
0.50	$\ u_h - U_h\ $	9.5288E-04	2.3690E-04	5.7849E-05	1.3876E-05	2.03 (2.0)
	$\ z_h - Z_h\ $	2.8092E-03	7.3280E-04	1.9346E-04	5.2271E-05	1.92 (2.0)
	$\ q_h - Q_h\ $	2.8092E-03	7.3280E-04	1.9346E-04	5.2271E-05	1.92 (2.0)
0.70	$\ u_h - U_h\ $	1.4006E-03	3.4003E-04	8.2500E-05	1.9979E-05	2.04 (2.0)
	$\ z_h - Z_h\ $	2.5076E-03	6.4431E-04	1.6911E-04	4.5804E-05	1.92 (2.0)
	$\ q_h - Q_h\ $	2.5076E-03	6.4431E-04	1.6911E-04	4.5804E-05	1.92 (2.0)
0.90	$\ u_h - U_h\ $	1.5531E-03	3.6841E-04	8.9197E-05	2.1787E-05	2.05 (2.0)
	$\ z_h - Z_h\ $	2.3271E-03	5.9800E-04	1.5806E-04	4.3190E-05	1.92 (2.0)
	$\ q_h - Q_h\ $	2.3271E-03	5.9800E-04	1.5806E-04	4.3190E-05	1.92 (2.0)

6 Conclusion

In this paper, we concentrate on higher order approximation in time of the optimal control problem governed by a time-fractional diffusion equation. A Crank-Nicolson scheme is designed for the optimal control problem and the corresponding optimality conditions are derived simultaneously. The optimal solutions are represented by using techniques based on the Laplace transform and Cauchy's integral formula. Then we rigorously analyze the temporal error estimate of the proposed scheme. Some numerical results are reported to verify the efficiency of our method by applying the conjugate gradient method to the fully discretized optimization problem without control constraints, which is consistent with the theoretical assertion.

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Declarations

Competing interests The authors have not disclosed any competing interests.

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