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A PRIORI ERROR ESTIMATES FOR SPACE-TIME FINITE ELEMENT DISCRETIZATION OF PARABOLIC OPTIMAL CONTROL PROBLEMS PART II: PROBLEMS WITH CONTROL CONSTRAINTS*

DOMINIK MEIDNER† AND BORIS VEXLER‡

Abstract. This paper is the second part of our work on a priori error analysis for finite element discretizations of parabolic optimal control problems. In the first part [*SIAM J. Control Optim.*, 47 (2008), pp. 1150–1177] problems without control constraints were considered. In this paper we derive a priori error estimates for space-time finite element discretizations of parabolic optimal control problems with pointwise inequality constraints on the control variable. The space discretization of the state variable is done using usual conforming finite elements, whereas the time discretization is based on discontinuous Galerkin methods. For the treatment of the control discretization we discuss different approaches, extending techniques known from the elliptic case.

Key words. optimal control, parabolic equations, error estimates, finite elements, pointwise inequality constraints

AMS subject classifications. 49N10, 49M25, 65M15, 65M60

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1. Introduction.

In this paper we develop a priori error analysis for space-time finite element discretizations of parabolic optimization problems. We consider the following linear-quadratic optimal control problem for the state variable u and the control variable q involving pointwise control constraints:

$$\text{Minimize } J(q,u) = \frac{1}{2}\int_0^T\int_\Omega (u(t,x)-\hat{u}(t,x))^2\,dx\,dt + \frac{\alpha}{2}\int_0^T\int_\Omega q(t,x)^2\,dx\,dt \tag{1.1a}$$

subject to

$$\begin{aligned} \partial_t u - \Delta u &= f + q \qquad \text{in } (0,T)\times\Omega, \\ u(0) &= u_0 \qquad \text{in } \Omega \end{aligned} \tag{1.1b}$$

and subject to

$$q_a \le q(t,x) \le q_b \quad \text{a.e. in } (0,T)\times\Omega, \tag{1.1c}$$

combined with either homogeneous Dirichlet or homogeneous Neumann boundary conditions on $(0,T)\times\partial\Omega$. A precise formulation of this problem including a functional analytic setting is given in the next section.

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http://www.siam.org/journals/sicon/47-3/69402.html
†Institut für Angewandte Mathematik, Ruprecht-Karls-Universität Heidelberg, INF 294, 69120 Heidelberg, Germany (dominik.meidner@iwr.uni-heidelberg.de).
‡Johann Radon Institute for Computational and Applied Mathematics (RICAM), Austrian Academy of Sciences, Altenberger Straße 69, 4040 Linz, Austria (boris.vexler@oeaw.ac.at).

Although the a priori error analysis for finite element discretization of optimal control problems governed by elliptic equations is discussed in many publications (see, e.g., [10, 12, 1, 13, 21, 7]), there are only a few published results on this topic for parabolic problems; see [19, 28, 16, 18, 23].

In the first part of our work on a priori error analysis of parabolic optimal control problems [20], we developed a priori error estimates for problems without control constraints. The consideration of control constraints (1.1c) leads to many additional difficulties. In the absence of inequality constraints the regularity of the optimal solution $(\bar{q}, \bar{u})$ of (1.1a)–(1.1b) is restricted only by the regularity of the domain Ω; by the regularity of the data $f, u_0, \hat{u}$; and possibly by some compatibility conditions. Therefore, in this case it is reasonable to assume high regularity of $(\bar{q}, \bar{u})$ leading to a corresponding order of convergence of the finite element discretization; see the discussion in [20].

The presence of control constraints (1.1c) leads to a stronger restriction of the regularity of the optimal solution, which is often reflected in a reduction of the order of convergence of the finite element discretization. For a discussion of the regularity of solutions to parabolic optimal control problems with control constraints, we refer, e.g., to [15].

In order to describe the claims and challenges of a priori error analysis for finite element discretization of (1.1), we first recall some corresponding results in the elliptic case. Using a finite element discretization with discretization parameter h, one can define a discretized optimal control problem with the discrete solution $(\bar{q}_h, \bar{u}_h)$.

Many authors made an effort to analyze the behavior of $\|\bar{q} - \bar{q}_h\|_{L^2(\Omega)}$ with respect to h: In the first papers concerning approximation of elliptic optimal control problems (see [10, 12]), the convergence order $\mathcal{O}(h)$ was established using a cellwise constant discretization of the control variable; see also [8, 1, 7]. For finite element discretization of the control variable by (bi-/tri-)linear H^1-conforming elements, the convergence order $\mathcal{O}(h^{\frac{3}{2}})$ can be shown; see, e.g., [5, 24, 2]. Recently, two approaches achieving $\mathcal{O}(h^2)$-convergence for the error in the control variable have been established; see [13, 21]. In [13] a *variational approach* is proposed, where no explicit discretization of the control variable is used. The discrete control variable is obtained by the projection of the discretized adjoint state on the set of admissible controls. In [21] a cellwise constant discretization is utilized, and a *postprocessing step* is used to obtain the desired accuracy. The latter technique is extended to optimal control of the Stokes equations in [25].

For discretization of parabolic problems such as (1.1), the state variable has to be discretized with respect to space and time leading to two discretization parameters h, k; see section 3 for a detailed description. The solution of the discretized optimal control problem is denoted by $(\bar{q}_\sigma, \bar{u}_\sigma)$, where $\sigma = (k, h, d)$ is a general discretization parameter and d denotes an abstract discretization parameter for the control space; cf. [20].

The main purpose of this paper is to analyze the behavior of $\|\bar{q} - \bar{q}_\sigma\|_{L^2(0,T;L^2(\Omega))}$ with respect to all involved discretization parameters. Our aim is to discuss the following four approaches for the discretization of the control variable, which extend some techniques known from the elliptic case:

1. Discretization using cellwise constant ansatz functions with respect to space and time. In this case we obtain, similar to [16, 18], the order of convergence $\mathcal{O}(h + k)$: The result is obtained under weaker regularity assumptions than

in [16, 18]. Moreover, we separate the influences of the spatial and temporal regularity on the discretization error; see Corollary 5.3.

2. Discretization using cellwise (bi-/tri-)linear, H^1-conforming finite elements in space, and piecewise constant functions in time: For this type of discretization we obtain the improved order of convergence $\mathcal{O}(k+h^{\frac{3}{2}-\frac{1}{p}})$; see Corollary 5.8. Here, p depends on the regularity of the adjoint solution. In two space dimensions we show the assertion for any $p < \infty$, whereas in three space dimensions the result is proved for $p \leq 6$. Under an additional regularity assumption, one can choose $p = \infty$ leading to $\mathcal{O}(k + h^{\frac{3}{2}})$. Again the influences of spatial and temporal regularity as well as of spatial and temporal discretization are clearly separated.
3. The discretization following the variational approach from [13], where no explicit discretization of the control variable is used: In this case we obtain an optimal result $\mathcal{O}(k + h^2)$; see Corollary 5.11. The usage of this approach requires a nonstandard implementation and more involved stopping criteria for optimization algorithms, since the control variable does not lie in any finite element space associated with the given mesh. However, there are no additional difficulties caused by the time discretization.
4. The postprocessing strategy extending the technique from [21] to parabolic problems: In this case we use the cellwise constant ansatz functions with respect to space and time. For the discrete solution $(\bar{q}_\sigma, \bar{u}_\sigma)$, a postprocessing step based on a projection formula is proposed leading to an approximation $\tilde{q}_\sigma$ with order of convergence $\|\bar{q} - \tilde{q}_\sigma\|_{L^2(0,T;L^2(\Omega))} = \mathcal{O}(k + h^{2-\frac{1}{p}})$; see Corollary 5.17. Here, p can be chosen as discussed for the cellwise linear discretization. Under an additional regularity assumption, one can also choose $p = \infty$ leading to $\mathcal{O}(k + h^2)$.

The paper is organized as follows. In the next section, we present a functional analytic setting for the optimal control problem (1.1) and discuss optimality conditions and the regularity of optimal solutions. Section 3 is devoted to the discretization of the considered optimal control problem. Therein, we address the temporal and spatial discretizations of the state equation by Galerkin finite element methods. Moreover, we give a detailed presentation of the four possibilities for discretizing the control variable introduced above. In section 4 we provide basic results on stability and approximation quality proved in the first part of this article [20]. In section 5 we develop our main results on a priori error analysis for the four mentioned types of control discretizations. Finally, we illustrate our theoretical results by numerical experiments.

2. Optimization. In this section we briefly discuss the precise formulation of the optimization problem under consideration. Furthermore, we recall theoretical results on existence, uniqueness, and regularity of optimal solutions as well as optimality conditions.

To set up a weak formulation of the state equation (1.1b), we introduce the following notation: For a convex polygonal domain $\Omega \subset \mathbb{R}^n$, $n = 2, 3$, we denote V to be either $H^1(\Omega)$ or $H^1_0(\Omega)$ depending on the prescribed type of boundary conditions (homogeneous Neumann or homogeneous Dirichlet). Together with $H = L^2(\Omega)$, the Hilbert space V and its dual V^* build a Gelfand triple $V \hookrightarrow H \hookrightarrow V^*$. Here and in what follows, we employ the usual notion for Lebesgue and Sobolev spaces.

For a time interval $I = (0, T)$ we introduce the state space

$$X := \{v | v \in L^2(I, V) \text{ and } \partial_t v \in L^2(I, V^*)\}$$

and the control space

$$Q = L^2(I, L^2(\Omega)).$$

In addition, we use the following notation for the inner products and norms on $L^2(\Omega)$ and $L^2(I, L^2(\Omega))$:

$$(v, w) := (v, w)_{L^2(\Omega)}, \qquad (v, w)_I := (v, w)_{L^2(I,L^2(\Omega))},$$
$$\|v\| := \|v\|_{L^2(\Omega)}, \qquad \|v\|_I := \|v\|_{L^2(I,L^2(\Omega))}.$$

In this setting, a standard weak formulation of the state equation (1.1b) for given control $q \in Q$, $f \in L^2(I, H)$, and $u_0 \in V$ reads as follows: Find a state $u \in X$ satisfying

$$\begin{aligned} (\partial_t u, \varphi)_I + (\nabla u, \nabla \varphi)_I &= (f + q, \varphi)_I \qquad \forall \varphi \in X, \\ u(0) &= u_0. \end{aligned} \tag{2.1}$$

As in Proposition 2.1 in [20] the following result on existence and regularity holds.

Proposition 2.1. *For fixed control $q \in Q$, $f \in L^2(I, H)$, and $u_0 \in V$ there exists a unique solution $u \in X$ of problem* (2.1)*. Moreover, the solution exhibits the improved regularity*

$$u \in L^2(I, H^2(\Omega) \cap V) \cap H^1(I, L^2(\Omega)) \hookrightarrow C(\bar{I}, V).$$

Furthermore, the stability estimate

$$\|\partial_t u\|_I + \|\nabla^2 u\|_I \le C\big\{\|f + q\|_I + \|\nabla u_0\|\big\}$$

holds.

To formulate the optimal control problem we introduce the admissible set Q_{ad}, collecting the inequality constraints (1.1c) as

$$Q_{\text{ad}} := \{q \in Q | q_a \le q(t, x) \le q_b \quad \text{a.e. in } I \times \Omega\},$$

where the bounds $q_a, q_b \in \mathbb{R}$ fulfill $q_a < q_b$.

The weak formulation of the optimal control problem (1.1) is given as follows:

$$\text{Minimize } J(q, u) := \frac{1}{2}\|u - \hat{u}\|_I^2 + \frac{\alpha}{2}\|q\|_I^2 \text{ subject to (2.1) and } (q, u) \in Q_{\text{ad}} \times X, \tag{2.2}$$

where $\hat{u} \in L^2(I, H)$ is a given desired state and $\alpha > 0$ is the regularization parameter.

Proposition 2.2. *For given $f, \hat{u} \in L^2(I, H)$, $u_0 \in V$, and $\alpha > 0$ the optimal control problem* (2.2) *admits a unique solution $(\bar{q}, \bar{u}) \in Q_{ad} \times X$.*

For the standard proof we refer, e.g., to [17].

The existence result for the state equation in Proposition 2.1 ensures the existence of a control-to-state mapping $q \mapsto u = u(q)$ defined through (2.1). By means of this mapping we introduce the reduced cost functional $j : Q \to \mathbb{R}$:

$$j(q) := J(q, u(q)).$$

The optimal control problem (2.2) can then be equivalently reformulated as follows:

$$\text{Minimize } j(q) \text{ subject to } q \in Q_{\text{ad}}. \tag{2.3}$$

The first order necessary optimality condition for (2.3) reads as

$$j'(\bar{q})(\delta q - \bar{q}) \geq 0 \quad \forall \delta q \in Q_{\mathrm{ad}}. \tag{2.4}$$

Due to the linear-quadratic structure of the optimal control problem, this condition is also sufficient for optimality.

Utilizing the adjoint state equation for $z = z(q) \in X$ given by

$$\begin{aligned} -(\varphi, \partial_t z)_I + (\nabla\varphi, \nabla z)_I &= (\varphi, u(q) - \hat{u})_I \qquad \forall \varphi \in X, \\ z(T) &= 0, \end{aligned} \tag{2.5}$$

the first derivative of the reduced cost functional can be expressed as

$$j'(q)(\delta q) = (\alpha q + z(q), \delta q)_I. \tag{2.6}$$

The second derivative $j''(q)(\cdot,\cdot)$ is independent of q and positive definite, i.e.,

$$j''(q)(p,p) \geq \alpha \|p\|_I^2 \quad \forall p \in Q. \tag{2.7}$$

Using a pointwise projection on the admissible set Q_{ad},

$$P_{Q_{\mathrm{ad}}} \colon Q \to Q_{\mathrm{ad}}, \quad P_{Q_{\mathrm{ad}}}(r)(t,x) = \max(q_a, \min(q_b, r(t,x))), \tag{2.8}$$

the optimality condition (2.4) can be expressed as

$$\bar{q} = P_{Q_{\mathrm{ad}}}\left(-\frac{1}{\alpha} z(\bar{q})\right). \tag{2.9}$$

It is well known that the projection $P_{Q_{\mathrm{ad}}}$ possesses the following property:

(2.10)
$$\|\nabla(P_{Q_{\mathrm{ad}}}(v))(t)\|_{L^p(\Omega)} \leq \|\nabla v(t)\|_{L^p(\Omega)} \quad \forall v \in L^2(I, W^{1,p}(\Omega)) \text{ and for a.a. } t \in I.$$

Employing formulation (2.9) of the optimality condition, we obtain the following regularity result.

PROPOSITION 2.3. *Let* $(\bar{q}, \bar{u})$ *be the solution of the optimization problem* (2.2) *and* $\bar{z} = z(\bar{q})$ *be the corresponding adjoint state. Then there holds*

$$\bar{u}, \bar{z} \in L^2(I, H^2(\Omega)) \cap H^1(I, L^2(\Omega)),$$

$$\bar{q} \in L^2(I, W^{1,p}(\Omega)) \cap H^1(I, L^2(\Omega)) \cap L^\infty(I \times \Omega)$$

for any $p < \infty$ *when* $n = 2$ *and* $p \leq 6$ *when* $n = 3$.

Proof. The regularity of $\bar{u}, \bar{z}$ follows directly from Proposition 2.1. The embedding $H^2(\Omega) \hookrightarrow W^{1,p}(\Omega)$ and property (2.10) imply the desired result for $\bar{q}$. ∎

3. Discretization. In this section we describe the space-time finite element discretization of optimal control problem (2.2).

3.1. Semidiscretization in time. At first, we present the semidiscretization in time of the state equation by discontinuous Galerkin methods following along the lines of the first part of this article [20]. We consider a partitioning of the time interval $\bar{I} = [0,T]$ as

$$\bar{I} = \{0\} \cup I_1 \cup I_2 \cup \cdots \cup I_M \tag{3.1}$$

with subintervals $I_m = (t_{m-1}, t_m]$ of size k_m and time points

$$0 = t_0 < t_1 < \cdots < t_{M-1} < t_M = T.$$

We define the discretization parameter k as a piecewise constant function by setting $k\big|_{I_m} = k_m$ for $m = 1, 2, \ldots, M$. Moreover, we denote by k the maximal size of the time steps, i.e., $k = \max k_m$.

The semidiscrete trial and test space is given as

$$X_k^r = \left\{ v_k \in L^2(I, V) | v_k\big|_{I_m} \in \mathcal{P}_r(I_m, V),\ m = 1, 2, \ldots, M \right\}.$$

Here, $\mathcal{P}_r(I_m, V)$ denotes the space of polynomials up to order r defined on I_m with values in V. On X_k^r we use the notation

$$(v, w)_{I_m} := (v, w)_{L^2(I_m, L^2(\Omega))} \quad \text{and} \quad \|v\|_{I_m} := \|v\|_{L^2(I_m, L^2(\Omega))}.$$

To define the discontinuous Galerkin approximation (dG(r)) using the space X_k^r, we employ the following definition for functions $v_k \in X_k^r$:

$$v_{k,m}^+ := \lim_{t \to 0^+} v_k(t_m + t), \quad v_{k,m}^- := \lim_{t \to 0^+} v_k(t_m - t) = v_k(t_m), \quad [v_k]_m := v_{k,m}^+ - v_{k,m}^-$$

and define the bilinear form $B(\cdot, \cdot)$ for $u_k, \varphi \in X_k^r$ by

$$B(u_k, \varphi) := \sum_{m=1}^{M} (\partial_t u_k, \varphi)_{I_m} + (\nabla u_k, \nabla \varphi)_I + \sum_{m=2}^{M} ([u_k]_{m-1}, \varphi_{m-1}^+) + (u_{k,0}^+, \varphi_0^+). \tag{3.2}$$

Then, the dG(r) semidiscretization of the state equation (2.1) for given control $q \in Q$ reads as follows: Find a state $u_k = u_k(q) \in X_k^r$ such that

$$B(u_k, \varphi) = (f + q, \varphi)_I + (u_0, \varphi_0^+) \quad \forall \varphi \in X_k^r. \tag{3.3}$$

The existence and uniqueness of solutions to (3.3) can be shown by using Fourier analysis; see [27] for details.

Remark 3.1. Using a density argument, it is possible to show that the exact solution $u = u(q) \in X$ satisfies the identity

$$B(u, \varphi) = (f + q, \varphi)_I + (u_0, \varphi_0^+) \quad \forall \varphi \in X_k^r.$$

Thus, we have here the property of Galerkin orthogonality

$$B(u - u_k, \varphi) = 0 \quad \forall \varphi \in X_k^r,$$

although the dG(r) semidiscretization is a nonconforming Galerkin method ($X_k^r \not\subset X$).

Throughout the paper we restrict ourselves to the case $r = 0$. The resulting dG(0) scheme is a variant of the implicit Euler method. In this case the semidiscrete state equation (3.3) can be explicitly rewritten as the following time-stepping scheme, using the fact that u_k is piecewise constant in time. We use the notation $U_m = u_k\big|_{I_m} \in V$ and obtain

$$(U_1, \psi) + k_1(\nabla U_1, \nabla \psi) = (f + q, \psi)_{I_m} + (u_0, \psi) \qquad \forall \psi \in V,$$

$$(U_m, \psi) + k_m(\nabla U_m, \nabla \psi) = (f + q, \psi)_{I_m} + (U_{m-1}, \psi) \qquad \forall \psi \in V,\ m = 2, 3, \ldots, M.$$

The semidiscrete optimization problem for the dG(0) time discretization has the following form:

$$\text{Minimize } J(q_k, u_k) \text{ subject to (3.3) and } (q_k, u_k) \in Q_{\text{ad}} \times X_k^0. \tag{3.4}$$

As in Proposition 3.2 in [20] the following result holds.

PROPOSITION 3.2. *For $\alpha > 0$, the semidiscrete optimal control problem* (3.4) *admits a unique solution $(\bar{q}_k, \bar{u}_k) \in Q_{ad} \times X_k^0$.*

Note that the optimal control $\bar{q}_k$ is searched for in the subset Q_{ad} of the continuous space Q, and the subscript k indicates the usage of the semidiscretized state equation.

Similarly to the continuous case, we introduce the semidiscrete reduced cost functional $j_k \colon Q \to \mathbb{R}$:

$$j_k(q) := J(q, u_k(q))$$

and reformulate the semidiscrete optimal control problem (3.4) as follows:

$$\text{Minimize } j_k(q_k) \text{ subject to } q_k \in Q_{\text{ad}}.$$

The first order necessary optimality condition reads as

$$j_k'(\bar{q}_k)(\delta q - \bar{q}_k) \geq 0 \quad \forall \delta q \in Q_{\text{ad}}, \tag{3.5}$$

and the derivative of j_k can be expressed as

$$j_k'(q)(\delta q) = (\alpha q + z_k(q), \delta q)_I. \tag{3.6}$$

Here, $z_k = z_k(q) \in X_k^0$ denotes the solution of the semidiscrete adjoint equation

$$B(\varphi, z_k) = (\varphi, u_k(q) - \hat{u})_I \quad \forall \varphi \in X_k^0. \tag{3.7}$$

As on the continuous level, the second derivative $j_k''(q)$ is independent of q and positive definite, i.e.,

$$j_k''(q)(p, p) \geq \alpha \|p\|_I^2 \quad \forall p \in Q. \tag{3.8}$$

Similarly to (2.9), the optimality condition (3.5) can be rewritten as

$$\bar{q}_k = P_{Q_{\text{ad}}} \left(-\frac{1}{\alpha} z_k(\bar{q}_k) \right). \tag{3.9}$$

This projection formula implies particularly that the optimal solution $\bar{q}_k$ is piecewise constant in time. We will make use of this fact in section 5.

3.2. Discretization in space. To define the finite element discretization in space, we consider two or three dimensional shape-regular meshes; see, e.g., [9]. A mesh consists of quadrilateral or hexahedral cells K, which constitute a non-overlapping cover of the computational domain Ω. The corresponding mesh is denoted by $\mathcal{T}_h = \{K\}$, where we define the discretization parameter h as a cellwise constant function by setting $h\big|_K = h_K$ with the diameter h_K of the cell K. We use the symbol h also for the maximal cell size, i.e., $h = \max h_K$.

On the mesh $\mathcal{T}_h$ we construct a conform finite element space $V_h \subset V$ in a standard way:

$$V_h^s = \left\{ v \in V | v\big|_K \in \mathcal{Q}_s(K) \text{ for } K \in \mathcal{T}_h \right\}.$$

Here, $\mathcal{Q}_s(K)$ consists of shape functions obtained via (bi-/tri-)linear transformations of polynomials in $\widehat{\mathcal{Q}_s}(\widehat{K})$ defined on the reference cell $\widehat{K} = (0,1)^n$; cf. section 3.2 in [20].

To obtain the fully discretized versions of the time discretized state equation (3.3), we utilize the space-time finite element space

$$X_{k,h}^{r,s} = \left\{ v_{kh} \in L^2(I, V_h^s) | v_{kh}\big|_{I_m} \in \mathcal{P}_r(I_m, V_h^s) \right\} \subset X_k^r.$$

Remark 3.3. Here, the spatial mesh, and therefore also the space V_h^s, is fixed for all time intervals. We refer to [26] for a discussion of treatment of different meshes $\mathcal{T}_h^m$ for each of the subintervals I_m.

The so-called cG(s)dG(r) discretization of the state equation for given control $q \in Q$ has the following form: Find a state $u_{kh} = u_{kh}(q) \in X_{k,h}^{r,s}$ such that

$$B(u_{kh}, \varphi) = (f + q, \varphi)_I + (u_0, \varphi_0^+) \quad \forall \varphi \in X_{k,h}^{r,s}. \tag{3.10}$$

Throughout this paper we will restrict ourselves to the consideration of (bi-/tri-)linear elements, i.e., we set $s = 1$ and consider the cG(1)dG(0) scheme.

Then, the corresponding optimal control problem is given as follows:

$$\text{Minimize } J(q_{kh}, u_{kh}) \text{ subject to (3.10) and } (q_{kh}, u_{kh}) \in Q_{\text{ad}} \times X_{k,h}^{0,1}, \tag{3.11}$$

and by means of the discrete reduced cost functional $j_{kh} \colon Q \to \mathbb{R}$,

$$j_{kh}(q) \coloneqq J(q, u_{kh}(q)),$$

it can be reformulated as follows:

$$\text{Minimize } j_{kh}(q_{kh}) \text{ subject to } q_{kh} \in Q_{\text{ad}}.$$

The uniquely determined optimal solution of (3.11) is denoted by $(\bar{q}_{kh}, \bar{u}_{kh}) \in Q_{\text{ad}} \times X_{k,h}^{0,1}$.

The optimal control $\bar{q}_{kh} \in Q_{\text{ad}}$ fulfills the first order optimality condition

$$j'_{kh}(\bar{q}_{kh})(\delta q - \bar{q}_{kh}) \geq 0 \quad \forall \delta q \in Q_{\text{ad}}, \tag{3.12}$$

where $j'_{kh}(q)(\delta q)$ is given by

$$j'_{kh}(q)(\delta q) = (\alpha q + z_{kh}(q), \delta q)_I \tag{3.13}$$

with the discrete adjoint solution $z_{kh} = z_{kh}(q) \in X_{k,h}^{0,1}$ of

$$B(\varphi, z_{kh}) = (\varphi, u_{kh}(q) - \hat{u})_I \quad \forall \varphi \in X_{k,h}^{0,1}. \tag{3.14}$$

For the second derivative of j_{kh} we have, as before,

$$j''_{kh}(q)(p, p) \geq \alpha \|p\|_I^2 \quad \forall p \in Q. \tag{3.15}$$

3.3. Discretization of the controls. In this subsection, we describe four different approaches for the discretization of the control variable. Choosing a subspace $Q_d \subset Q$, we introduce the corresponding admissible set

$$Q_{d,\text{ad}} = Q_d \cap Q_{\text{ad}}.$$

Note that in what follows, the space Q_d will be either finite dimensional or the whole space Q. The optimal control problem on this level of discretization is given as follows:

$$\text{Minimize } J(q_\sigma, u_\sigma) \text{ subject to (3.10) and } (q_\sigma, u_\sigma) \in Q_{d,\text{ad}} \times X_{k,h}^{0,1}. \tag{3.16}$$

The unique optimal solution of (3.16) is denoted by $(\bar{q}_\sigma, \bar{u}_\sigma) \in Q_{d,\text{ad}} \times X_{k,h}^{0,1}$, where the subscript σ collects the discretization parameters k, h, and d. The optimality condition is given using the discrete reduced cost functional j_{kh} introduced before:

$$j'_{kh}(\bar{q}_\sigma)(\delta q - \bar{q}_\sigma) \geq 0 \quad \forall \delta q \in Q_{d,\text{ad}}. \tag{3.17}$$

3.3.1. Cellwise constant discretization. The first possibility for the control discretization is to use cellwise constant functions. Employing the same time partitioning and the same spatial mesh as for the discretization of the state variable, we set

$$Q_d = \left\{ q \in Q | q\big|_{I_m \times K} \in \mathcal{P}_0(I_m \times K),\ m = 1, 2, \dots, M,\ K \in \mathcal{T}_h \right\}.$$

The discretization error for this type of discretization will be analyzed in section 5.1.

3.3.2. Cellwise linear discretization. Another possibility for the discretization of the control variable is to choose the same control discretization as for the state variable, i.e., piecewise constant in time and cellwise (bi-/tri-)linear in space. Using a spatial space

$$Q_h = \left\{ v \in C(\bar{\Omega}) | v\big|_K \in \mathcal{Q}_1(K) \text{ for } K \in \mathcal{T}_h \right\},$$

we set

$$Q_d = \left\{ q \in Q | q\big|_{I_m} \in \mathcal{P}_0(I_m, Q_h) \right\}.$$

The state space $X_{k,h}^{0,1}$ coincides with the control space Q_d in the case of homogeneous Neumann boundary conditions and is a subspace of it, i.e., $Q_d \supset X_{k,h}^{0,1}$ in the presence of homogeneous Dirichlet boundary conditions.

The discretization error for this type of discretization will be analyzed in section 5.2.

3.3.3. Variational approach. Extending the discretization approach presented in [13], we can choose $Q_d = Q$. In this case the optimization problems (3.11) and (3.16) coincide, and therefore $\bar{q}_\sigma = \bar{q}_{kh} \in Q_{\text{ad}}$.

We use the fact that the optimality condition (3.12) can be rewritten employing the projection (2.8) as

$$\bar{q}_{kh} = P_{Q_{\text{ad}}} \left(-\frac{1}{\alpha} z_{kh}(\bar{q}_{kh}) \right),$$

and we obtain that $\bar{q}_{kh}$ is a piecewise constant function in time. However, $\bar{q}_{kh}$ is in general not a finite element function corresponding to the spatial mesh $\mathcal{T}_h$. This fact requires more care for the construction of algorithms for computation of $\bar{q}_{kh}$; see [13] for details.

The discretization error for this type of discretization will be analyzed in section 5.3.

3.3.4. Postprocessing strategy. The strategy described in this section extends the approach from [21] to parabolic problems. For the discretization of the control space we employ the same choice as in section 3.3.1, i.e., cellwise constant discretization. After the computation of the corresponding solution $\bar{q}_\sigma$, a better approximation $\tilde{q}_\sigma$ is constructed by a postprocessing, making use of the projection operator (2.8):

$$\tilde{q}_\sigma = P_{Q_{\mathrm{ad}}}\left(-\frac{1}{\alpha} z_{kh}(\bar{q}_\sigma)\right). \tag{3.18}$$

Note that, similar to the solution obtained by the variational approach in section 3.3.3, the solution $\tilde{q}_\sigma$ is piecewise constant in time and is generally not a finite element function in space with respect to the spatial mesh $\mathcal{T}_h$. This solution can be simply evaluated pointwise; however, the corresponding error analysis requires an additional assumption on the structure of active sets; see the discussion in section 5.4.

4. Auxiliary results. In this section we recall some results provided in the first part of this article [20], which will be used in what follows.

The first proposition provides a stability result for the purely time discretized state and adjoint solutions. It follows from Theorems 4.1 and 4.3 and Corollaries 4.2 and 4.5 of [20] as well as from elliptic regularity.

PROPOSITION 4.1. *For $q \in Q$ let the solutions $u_k(q) \in X_k^0$ and $z_k(q) \in X_k^0$ be given by the semidiscrete state equation* (3.3) *and adjoint equation* (3.7)*, respectively. Then it holds that*

$$\|\nabla^2 u_k(q)\|_I + \|\nabla u_k(q)\|_I + \|u_k(q)\|_I \le C\big\{\|f + q\|_I + \|\nabla u_0\| + \|u_0\|\big\},$$

$$\|\nabla^2 z_k(q)\|_I + \|\nabla z_k(q)\|_I + \|z_k(q)\|_I \le C\|u_k(q) - \hat{u}\|_I.$$

A similar result holds for the fully discretized solutions of the state and adjoint equations; cf. Theorem 4.6 and Corollary 4.7 in [20].

PROPOSITION 4.2. *For $q \in Q$ let the solutions $u_{kh}(q) \in X_{k,h}^{0,1}$ and $z_{kh}(q) \in X_{k,h}^{0,1}$ be given by the discrete state equation* (3.10) *and adjoint equation* (3.14)*, respectively. Then it holds that*

$$\|\nabla u_{kh}(q)\|_I + \|u_{kh}(q)\|_I \le C\big\{\|f + q\|_I + \|\nabla \Pi_h u_0\| + \|\Pi_h u_0\|\big\},$$

$$\|\nabla z_{kh}(q)\|_I + \|z_{kh}(q)\|_I \le C\|u_{kh}(q) - \hat{u}\|_I,$$

where $\Pi_h \colon V \to V_h$ denotes the spatial L^2-projection.

In the following two propositions, we recall a priori estimates for the errors due to temporal and spatial discretizations of the state and adjoint variables. The assertions are proved in [20] by means of Theorems 5.1 and 5.5 as well as by Lemma 6.2 presented therein.

PROPOSITION 4.3. *For $q \in Q$ let the solutions $u(q) \in X$ and $z(q) \in X$ be given by the state equation* (2.1) *and adjoint equation* (2.5)*, respectively. Moreover, let $u_k(q) \in X_k^0$ and $z_k(q) \in X_k^0$ be determined as solutions of the semidiscrete state equation* (3.3) *and adjoint equation* (3.7)*. Then the following error estimates hold:*

$$\|u(q) - u_k(q)\|_I \le Ck\|\partial_t u(q)\|_I,$$

$$\|z(q) - z_k(q)\|_I \le Ck\big\{\|\partial_t u(q)\|_I + \|\partial_t z(q)\|_I\big\}.$$

PROPOSITION 4.4. *For $q \in Q$ let the solutions $u_k(q) \in X_k^0$ and $z_k(q) \in X_k^0$ be given by the semidiscrete state equation* (3.3) *and adjoint equation* (3.7)*, respectively.*

Moreover, let $u_{kh}(q) \in X^{0,1}_{k,h}$ *and* $z_{kh}(q) \in X^{0,1}_{k,h}$ *be determined as solutions of the discrete state equation* (3.10) *and adjoint equation* (3.14). *Then the following error estimates hold:*

$$\|u_k(q) - u_{kh}(q)\|_I \le Ch^2 \|\nabla^2 u_k(q)\|_I,$$

$$\|z_k(q) - z_{kh}(q)\|_I \le Ch^2 \big\{ \|\nabla^2 u_k(q)\|_I + \|\nabla^2 z_k(q)\|_I \big\}.$$

Proposition 4.2 provides a stability result for the discrete adjoint solution with respect to the norm of $L^2(I, H^1(\Omega))$. For later use we additionally prove a corresponding result with respect to the norm of $L^2(I, L^\infty(\Omega))$.

LEMMA 4.5. *For* $q \in Q$ *let the solutions* $u_{kh}(q) \in X^{0,1}_{k,h}$ *and* $z_{kh}(q) \in X^{0,1}_{k,h}$ *be given by the discrete state equation* (3.10) *and adjoint equation* (3.14), *respectively. Then it holds that*

$$\|z_{kh}(q)\|_{L^2(I,L^\infty(\Omega))} \le C \|u_{kh}(q) - \hat{u}\|_I.$$

Proof. We define an additional adjoint solution $\tilde{z}_k \in X^0_k$ as solution of

$$B(\varphi, \tilde{z}_k) = (\varphi, u_{kh}(q) - \hat{u})_I \quad \forall \varphi \in X^0_k.$$

Since $\tilde{z}_k$ and $z_{kh}(q)$ are given by means of the same right-hand side $u_{kh}(q) - \hat{u}$, it is possible to apply standard a priori error estimates to the discretization error $z_{kh}(q) - \tilde{z}_k$ similar to Proposition 4.4.

By inserting the solution $\tilde{z}_k$ and utilizing the embedding $L^2(I, H^2(\Omega)) \hookrightarrow L^2(I, L^\infty(\Omega))$, we get

$$\begin{aligned} \|z_{kh}(q)\|_{L^2(I,L^\infty(\Omega))} &\le \|z_{kh}(q) - \tilde{z}_k\|_{L^2(I,L^\infty(\Omega))} + \|\tilde{z}_k\|_{L^2(I,L^\infty(\Omega))} \\ &\le \|z_{kh}(q) - \tilde{z}_k\|_{L^2(I,L^\infty(\Omega))} + C\|\tilde{z}_k\|_{L^2(I,H^2(\Omega))}. \end{aligned}$$

For the first term we obtain, by inserting a spatial interpolation $i_h \tilde{z}_k \in X^{0,1}_{k,h}$,

$$\|z_{kh}(q) - \tilde{z}_k\|_{L^2(I,L^\infty(\Omega))} \le \|z_{kh}(q) - i_h \tilde{z}_k\|_{L^2(I,L^\infty(\Omega))} + \|i_h \tilde{z}_k - \tilde{z}_k\|_{L^2(I,L^\infty(\Omega))}. \tag{4.1}$$

For the first term on the right-hand side of (4.1) we proceed by means of an inverse estimate between $L^\infty(\Omega)$ and $L^2(\Omega)$ for discrete functions, an estimate for the error due to space discretization (cf. Theorem 5.1 of [20]), and an estimate for the spatial interpolation error as

$$\begin{aligned} \|z_{kh}(q) - i_h \tilde{z}_k\|^2_{L^2(I,L^\infty(\Omega))} &= \sum_{m=1}^{M} k_m \|z_{kh}(q)(t_m) - i_h \tilde{z}_k(t_m)\|^2_{L^\infty(\Omega)} \\ &\le Ch^{-n} \sum_{m=1}^{M} k_m \|z_{kh}(q)(t_m) - i_h \tilde{z}_k(t_m)\|^2 \\ &\le Ch^{-n} \big\{ \|z_{kh}(q) - \tilde{z}_k\|^2_I + \|\tilde{z}_k - i_h \tilde{z}_k\|^2_I \big\} \\ &\le Ch^{4-n} \|\nabla^2 \tilde{z}_k\|^2_I. \end{aligned}$$

By standard interpolation estimates, we have for the second term on the right-hand side of (4.1),

$$\begin{aligned}\|i_h\tilde{z}_k - \tilde{z}_k\|^2_{L^2(I,L^\infty(\Omega))} &= \sum_{m=1}^{M} k_m \|i_h\tilde{z}_k(t_m) - \tilde{z}_k(t_m)\|^2_{L^\infty(\Omega)} \\ &\le Ch^{4-n} \sum_{m=1}^{M} k_m \|\nabla^2 \tilde{z}_k(t_m)\|^2 \\ &= Ch^{4-n}\|\nabla^2\tilde{z}_k\|^2_I.\end{aligned}$$

We complete the proof by collecting all estimates and application of the stability result from Proposition 4.1:

$$\|z_{kh}(q)\|_{L^2(I,L^\infty(\Omega))} \le Ch^{4-n}\|\nabla^2\tilde{z}_k\|_I + C\|\tilde{z}_k\|_{L^2(I,H^2(\Omega))} \le C\|u_{kh}(q) - \hat{u}\|_I. \qquad \square$$

5. Error estimates. In this section we provide a priori error estimates for the different discretization approaches described in section 3. We start with an assertion of the error between the solution $\bar{q}$ of the continuous problem (2.2) and the solution $\bar{q}_k$ of the semidiscretized problem (3.4).

THEOREM 5.1. *Let $\bar{q} \in Q_{ad}$ be the solution of optimization problem* (2.2) *and $\bar{q}_k$ be the solution of the semidiscretized problem* (3.4)*. Then the following estimate holds:*

$$\|\bar{q} - \bar{q}_k\|_I \le \frac{1}{\alpha}\|z(\bar{q}) - z_k(\bar{q})\|_I.$$

Proof. Using the optimality conditions (2.4) and (3.5), we obtain the relation

$$-j_k'(\bar{q}_k)(\bar{q} - \bar{q}_k) \le 0 \le -j'(\bar{q})(\bar{q} - \bar{q}_k).$$

From (3.8) we have with any $p \in Q$:

$$\begin{aligned}\alpha\|\bar{q} - \bar{q}_k\|^2_I &\le j_k''(p)(\bar{q} - \bar{q}_k, \bar{q} - \bar{q}_k) \\ &= j_k'(\bar{q})(\bar{q} - \bar{q}_k) - j_k'(\bar{q}_k)(\bar{q} - \bar{q}_k) \\ &\le j_k'(\bar{q})(\bar{q} - \bar{q}_k) - j'(\bar{q})(\bar{q} - \bar{q}_k).\end{aligned}$$

By means of the representations (2.6) and (3.6) of j' and j_k', respectively, we obtain

$$\alpha\|\bar{q} - \bar{q}_k\|^2_I \le (z(\bar{q}) - z_k(\bar{q}), \bar{q} - \bar{q}_k)_I.$$

The desired assertion follows by Cauchy's inequality. $\square$

5.1. Cellwise constant discretization. In this section we are going to prove an estimate for the error $\|\bar{q} - \bar{q}_\sigma\|_I$ when the control is discretized by cellwise constant polynomials in space and time; see section 3.3.1.

For doing so, we will extend the techniques presented in [8] to the case of parabolic optimal control problems. This demands the introduction of the solution $\bar{q}_d$ of the following purely control discretized problem:

(5.1) $$\text{Minimize } j(q_d) \text{ subject to } q_d \in Q_{d,\text{ad}}.$$

The uniquely determined solution $\bar{q}_d$ fulfills the optimality condition

$$j'(\bar{q}_d)(\delta q - \bar{q}_d) \geq 0 \quad \forall \delta q \in Q_{d,\mathrm{ad}}. \tag{5.2}$$

To formulate the main result of this section, we introduce the L^2-projection $\pi_d \colon Q \to Q_d$ and note that, due to the cellwise constant discretization, the following property holds true:

$$\pi_d Q_{\mathrm{ad}} \subset Q_{d,\mathrm{ad}}.$$

THEOREM 5.2. *Let $\bar{q} \in Q_{ad}$ be the solution of the optimal control problem* (2.2), *and let $\bar{q}_\sigma \in Q_{d,ad}$ be the solution of the discretized problem* (3.16), *where the cellwise constant discretization for the control variable is employed. Moreover, let $\bar{q}_d \in Q_{d,ad}$ be the solution of the purely control discretized problem* (5.1). *Then the following estimate holds:*

$$\|\bar{q} - \bar{q}_\sigma\|_I \leq \|\bar{q} - \pi_d \bar{q}\|_I + \frac{1}{\alpha}\|z(\bar{q}_d) - \pi_d z(\bar{q}_d)\|_I + \frac{1}{\alpha}\|z(\bar{q}_d) - z_{kh}(\bar{q}_d)\|_I.$$

Proof. We split the error

$$\|\bar{q} - \bar{q}_\sigma\|_I \leq \|\bar{q} - \bar{q}_d\|_I + \|\bar{q}_d - \bar{q}_\sigma\|_I$$

and estimate both terms on the right-hand side separately. For treating the first term, we use the fact that $\pi_d \bar{q} \in Q_{d,\mathrm{ad}}$ and obtain from the optimality conditions (2.4) and (5.2) the inequalities

$$j'(\bar{q})(\bar{q} - \bar{q}_d) \leq 0 \quad \text{and} \quad -j'(\bar{q}_d)(\pi_d \bar{q} - \bar{q}_d) \leq 0.$$

Using (2.7) we proceed with any $p \in Q$:

$$\begin{aligned}
\alpha\|\bar{q} - \bar{q}_d\|_I^2 &\leq j''(p)(\bar{q} - \bar{q}_d, \bar{q} - \bar{q}_d) \\
&= j'(\bar{q})(\bar{q} - \bar{q}_d) - j'(\bar{q}_d)(\bar{q} - \bar{q}_d) \\
&= j'(\bar{q})(\bar{q} - \bar{q}_d) - j'(\bar{q}_d)(\bar{q} - \pi_d \bar{q}) - j'(\bar{q}_d)(\pi_d \bar{q} - \bar{q}_d) \\
&\leq -j'(\bar{q}_d)(\bar{q} - \pi_d \bar{q}).
\end{aligned}$$

By means of the representation of the derivative j' from (2.6) and the properties of π_d, we have

$$\begin{aligned}
\alpha\|\bar{q} - \bar{q}_d\|_I^2 &\leq -j'(\bar{q}_d)(\bar{q} - \pi_d \bar{q}) \\
&= -(\alpha \bar{q}_d + z(\bar{q}_d), \bar{q} - \pi_d \bar{q})_I \\
&= (\pi_d z(\bar{q}_d) - z(\bar{q}_d), \bar{q} - \pi_d \bar{q})_I,
\end{aligned}$$

and by Young's inequality we obtain the intermediary result

$$\|\bar{q} - \bar{q}_d\|_I^2 \leq \|\bar{q} - \pi_d \bar{q}\|_I^2 + \frac{1}{4\alpha^2}\|z(\bar{q}_d) - \pi_d z(\bar{q}_d)\|_I^2. \tag{5.3}$$

In order to estimate the term $\|\bar{q}_d - \bar{q}_\sigma\|_I$ we exploit the optimality conditions (5.2) and (3.17) leading to the following relation:

$$-j'_{kh}(\bar{q}_\sigma)(\bar{q}_d - \bar{q}_\sigma) \leq 0 \leq -j'(\bar{q}_d)(\bar{q}_d - \bar{q}_\sigma).$$

Using (3.15) and the representations (2.6) for j' and (3.13) for j'_{kh}, respectively, we obtain

$$\begin{aligned}\alpha\|\bar q_d-\bar q_\sigma\|_I^2 &\le j''_{kh}(p)(\bar q_d-\bar q_\sigma,\bar q_d-\bar q_\sigma)\\ &= j'_{kh}(\bar q_d)(\bar q_d-\bar q_\sigma)-j'_{kh}(\bar q_\sigma)(\bar q_d-\bar q_\sigma)\\ &\le j'_{kh}(\bar q_d)(\bar q_d-\bar q_\sigma)-j'(\bar q_d)(\bar q_d-\bar q_\sigma)\\ &\le \|z(\bar q_d)-z_{kh}(\bar q_d)\|_I\|\bar q_d-\bar q_\sigma\|_I.\end{aligned}$$

Thus, we achieve

$$\|\bar q_d-\bar q_\sigma\|_I\le\frac{1}{\alpha}\|z(\bar q_d)-z_{kh}(\bar q_d)\|_I. \tag{5.4}$$

Collecting estimates (5.3) and (5.4), we complete the proof. ∎

This theorem directly implies the following result.

Corollary 5.3. *Under the conditions of Theorem* 5.2*, the following estimate holds:*

$$\begin{aligned}\|\bar q-\bar q_\sigma\|_I &\le \frac{C}{\alpha}\,k\left\{\|\partial_t\bar q\|_I+\|\partial_t u(\bar q_d)\|_I+\|\partial_t z(\bar q_d)\|_I\right\}\\ &\quad+\frac{C}{\alpha}\,h\left\{\|\nabla\bar q\|_I+\|\nabla z(\bar q_d)\|_I+h\left(\|\nabla^2 u_k(\bar q_d)\|_I+\|\nabla^2 z_k(\bar q_d)\|_I\right)\right\}=\mathcal{O}(k+h).\end{aligned}$$

Proof. The assertion follows from Theorem 5.2 by interpolation estimates and Propositions 4.3 and 4.4. Due to the fact that $\bar q,\bar q_d\in Q_{\mathrm{ad}}$, we obtain, using the stability estimates from Proposition 4.1, that all norms involved in this estimate are bounded by a constant independent of all discretization parameters. ∎

5.2. Cellwise linear discretization. This section is devoted to the error analysis for the discretization of the control variable by piecewise constants in time and cellwise (bi-/tri-)linear functions in space as described in section 3.3.2. To this end we split the error

$$\|\bar q-\bar q_\sigma\|_I\le\|\bar q-\bar q_k\|_I+\|\bar q_k-\bar q_\sigma\|_I$$

and use the result of Theorem 5.1 for the first part. For treating the error $\|\bar q_k-\bar q_\sigma\|_I$ we adapt the technique described in [4] and [6] to parabolic problems.

The analysis in this section is based on an assumption on the structure of the active sets. For each time interval I_m we group the cells K of the mesh $\mathcal{T}_h$ depending on the value of $\bar q_k$ on K into three sets $\mathcal{T}_h=\mathcal{T}_{h,m}^1\cup\mathcal{T}_{h,m}^2\cup\mathcal{T}_{h,m}^3$ with $\mathcal{T}_{h,m}^i\cap\mathcal{T}_{h,m}^j=\emptyset$ for $i\ne j$. The sets are chosen as follows:

$$\begin{aligned}\mathcal{T}_{h,m}^1&:=\left\{K\in\mathcal{T}_h\,|\,\bar q_k(t_m,x)=q_a\text{ or }\bar q_k(t_m,x)=q_b\quad\forall x\in K\right\},\\ \mathcal{T}_{h,m}^2&:=\left\{K\in\mathcal{T}_h\,|\,q_a<\bar q_k(t_m,x)<q_b\quad\forall x\in K\right\},\\ \mathcal{T}_{h,m}^3&:=\mathcal{T}_h\setminus(\mathcal{T}_{h,m}^1\cup\mathcal{T}_{h,m}^2).\end{aligned}$$

Hence, the set $\mathcal{T}_{h,m}^3$ consists of the cells which contain the free boundary between the active and the inactive sets for the time interval I_m.

Assumption 1. We assume that there exists a positive constant C independent of k, h, and m such that

$$\sum_{K\in\mathcal{T}^3_{h,m}} |K| \le Ch$$

separately for all $m = 1, 2, \ldots, M$.

Remark 5.4. A similar assumption is used in [21, 25, 2]. This assumption is valid if the boundary of the level sets

$$\{x \in \Omega | \bar{q}_k(t_m, x) = q_a\} \quad \text{and} \quad \{x \in \Omega | \bar{q}_k(t_m, x) = q_b\}$$

consists of a finite number of rectifiable curves.

We consider the usual nodal interpolation operator I_d which maps into the space of cellwise (bi-/tri-)linear functions Q_h. It is defined for functions $g \in C(\Omega)$ by pointwise setting

$$I_d g(x_i) = g(x_i) \quad \text{for each node } x_i \text{ of } \mathcal{T}_h. \tag{5.5}$$

The operator I_d will also be applied to time-dependent functions g by the setting $(I_d g)(t) = I_d g(t)$.

In the following theorem we provide an assertion on the error $\|\bar{q}_k - \bar{q}_\sigma\|_I$.

THEOREM 5.5. *Let $\bar{q}_k \in Q_{ad}$ be the solution of the semidiscretized optimal control problem* (3.4) *and $\bar{q}_\sigma \in Q_{d,ad}$ be the solution of the discrete problem* (3.16)*, where the cellwise (bi-/tri-)linear discretization for the control variable is employed. Then the following estimate holds:*

$$\|\bar{q}_k - \bar{q}_\sigma\|_I \le C\Big(1 + \frac{1}{\alpha}\Big)\|I_d\bar{q}_k - \bar{q}_k\|_I + \frac{C}{\alpha}\|z_k(\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I + \frac{C}{\sqrt{\alpha}}\big(j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k)\big)^{\frac{1}{2}}.$$

Proof. We split

$$\|\bar{q}_k - \bar{q}_\sigma\|_I \le \|\bar{q}_k - I_d\bar{q}_k\|_I + \|I_d\bar{q}_k - \bar{q}_\sigma\|_I \tag{5.6}$$

and estimate the term $\|I_d\bar{q}_k - \bar{q}_\sigma\|_I$. Due to the optimality conditions (3.17) and (3.5), and since $I_d\bar{q}_k \in Q_{d,\mathrm{ad}}$, we have

$$-j_{kh}'(\bar{q}_\sigma)(I_d\bar{q}_k - \bar{q}_\sigma) \le 0 \le -j_k'(\bar{q}_k)(\bar{q}_k - \bar{q}_\sigma),$$

and due to (3.15) we obtain for any $p \in Q$,

$$\begin{aligned}
\alpha\|I_d\bar{q}_k - \bar{q}_\sigma\|_I^2 &\le j_{kh}''(p)(I_d\bar{q}_k - \bar{q}_\sigma, I_d\bar{q}_k - \bar{q}_\sigma)\\
&\le j_{kh}'(I_d\bar{q}_k)(I_d\bar{q}_k - \bar{q}_\sigma) - j_{kh}'(\bar{q}_\sigma)(I_d\bar{q}_k - \bar{q}_\sigma)\\
&\le j_{kh}'(I_d\bar{q}_k)(I_d\bar{q}_k - \bar{q}_\sigma) - j_k'(\bar{q}_k)(\bar{q}_k - \bar{q}_\sigma)\\
&= j_{kh}'(I_d\bar{q}_k)(I_d\bar{q}_k - \bar{q}_\sigma) - j_{kh}'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_\sigma)\\
&\quad + j_{kh}'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_\sigma) - j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_\sigma)\\
&\quad + j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k).
\end{aligned} \tag{5.7}$$

The representations (3.6) of j_k' and (3.13) of j_{kh}' yield, by means of Proposition 4.2, that for any $p, q, r \in Q$,

$$|j_{kh}'(p)(r) - j_{kh}'(q)(r)| \leq \{\alpha\|p-q\|_I + \|z_{kh}(p) - z_{kh}(q)\|_I\}\|r\|_I \leq (C+\alpha)\|p-q\|_I\|r\|_I$$

and

$$|j_{kh}'(q)(r) - j_k'(q)(r)| \leq \|z_k(q) - z_{kh}(q)\|_I\|r\|_I.$$

Applying these inequalities to the right-hand side of (5.7) leads to

$$\begin{aligned}\alpha\|I_d\bar{q}_k - \bar{q}_\sigma\|_I^2 \leq (C+\alpha)\|I_d\bar{q}_k - \bar{q}_k\|_I\|I_d\bar{q}_k - \bar{q}_\sigma\|_I \\ + \|z_k(\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I\|I_d\bar{q}_k - \bar{q}_\sigma\|_I + j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k).\end{aligned}$$

With Young's inequality, we obtain

$$\begin{aligned}\|I_d\bar{q}_k - \bar{q}_\sigma\|_I^2 \leq C\Big(1 + \frac{1}{\alpha^2}\Big)\|I_d\bar{q}_k - \bar{q}_k\|_I^2 \\ + \frac{C}{\alpha^2}\|z_k(\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I^2 + \frac{C}{\alpha}j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k).\end{aligned}$$

Inserting this estimate into (5.6) completes the proof. □

In the following two lemmas we provide estimates for the terms $j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k)$ and $\|I_d\bar{q}_k - \bar{q}_k\|_I$ appearing on the right-hand side of the assertion of Theorem 5.5.

LEMMA 5.6. *Let $\bar{q}_k \in Q_{ad}$ be the solution of the semidiscretized optimization problem* (3.4) *and $I_d\bar{q}_k$ be the interpolation constructed by* (5.5)*. Then, if Assumption 1 is fulfilled, the following estimate holds for $n < p \leq \infty$, provided $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$:*

$$|j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k)| \leq \frac{C}{\alpha}h^{3-\frac{2}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))}^2.$$

Proof. Using representation (3.6) of j_k' we have

$$\begin{aligned}j_k'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k) &= (\alpha\bar{q}_k + z_k(\bar{q}_k), I_d\bar{q}_k - \bar{q}_k)_I \\ &= \sum_{m=1}^{M}\int_{I_m}(\alpha\bar{q}_k(t) + z_k(\bar{q}_k)(t), I_d\bar{q}_k(t) - \bar{q}_k(t))\,dt \\ &= \sum_{m=1}^{M}k_m(\alpha\bar{q}_k(t_m) + z_k(\bar{q}_k)(t_m), I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)).\end{aligned} \tag{5.8}$$

With the abbreviation $d_m := \alpha\bar{q}_k(t_m) + z_k(\bar{q}_k)(t_m)$ we obtain

$$\begin{aligned}(d_m, I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)) &= \sum_{K\in\mathcal{T}_h}(d_m, I_d\bar{q}_k(t_m) - \bar{q}_k(t_m))_{L^2(K)} \\ &= \sum_{K\in\mathcal{T}_{h,m}^3}(d_m, I_d\bar{q}_k(t_m) - \bar{q}_k(t_m))_{L^2(K)},\end{aligned} \tag{5.9}$$

since it holds $I_d\bar{q}_k(t_m) = \bar{q}_k(t_m)$ on $\mathcal{T}_{h,m}^1$ by construction and $d_m = 0$ on $\mathcal{T}_{h,m}^2$ due to representation formula (3.9).

In every cell $K \in \mathcal{T}^3_{h,m}$ there is a point x_K with $d_m(x_K) = 0$. Thus, we get

$$\begin{aligned}
&|(d_m, I_d\bar{q}_k(t_m) - \bar{q}_k(t_m))_{L^2(K)}| \\
&\qquad \le |K|^{1-\frac{2}{p}} \|d_m\|_{L^p(K)} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|_{L^p(K)} \\
&\qquad = |K|^{1-\frac{2}{p}} \|d_m - d_m(x_K)\|_{L^p(K)} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|_{L^p(K)} \\
&\qquad \le Ch^2 |K|^{1-\frac{2}{p}} \|\nabla d_m\|_{L^p(K)} \|\nabla\bar{q}_k(t_m)\|_{L^p(K)}.
\end{aligned}$$

Inserting this estimate into (5.9) yields, together with Assumption 1,

$$\begin{aligned}
|(d_m, I_d\bar{q}_k(t_m) - \bar{q}_k(t_m))| &\le Ch^2 \sum_{K \in \mathcal{T}^3_{h,m}} |K|^{1-\frac{2}{p}} \|\nabla d_m\|_{L^p(K)} \|\nabla\bar{q}_k(t_m)\|_{L^p(K)} \\
&\le Ch^2 \left(\sum_{K \in \mathcal{T}^3_{h,m}} |K| \right)^{1-\frac{2}{p}} \|\nabla d_m\|_{L^p(\Omega)} \|\nabla\bar{q}_k(t_m)\|_{L^p(\Omega)} \\
&\le Ch^{3-\frac{2}{p}} \|\nabla d_m\|_{L^p(\Omega)} \|\nabla\bar{q}_k(t_m)\|_{L^p(\Omega)}.
\end{aligned}$$

Then, the estimate

$$\|\nabla d_m\|_{L^p(\Omega)} \le \alpha \|\nabla q_k(\bar{q}_k)(t_m)\|_{L^p(\Omega)} + \|\nabla z_k(\bar{q}_k)(t_m)\|_{L^p(\Omega)},$$

representation formula (3.9), and property (2.10) imply

$$|(d_m, I_d\bar{q}_k(t_m) - \bar{q}_k(t_m))| \le \frac{C}{\alpha} h^{3-\frac{2}{p}} \|\nabla z_k(\bar{q}_k)(t_m)\|^2_{L^p(\Omega)}.$$

Hence, by inserting this last estimate into (5.8) we obtain the proposed assertion

$$\begin{aligned}
|j'(\bar{q}_k)(I_d\bar{q}_k - \bar{q}_k)| &\le \frac{C}{\alpha} h^{3-\frac{2}{p}} \sum_{m=1}^{M} k_m \|\nabla z_k(\bar{q}_k)(t_m)\|^2_{L^p(\Omega)} \\
&= \frac{C}{\alpha} h^{3-\frac{2}{p}} \|\nabla z_k(\bar{q}_k)\|^2_{L^2(I,L^p(\Omega))}. \qquad \square
\end{aligned}$$

LEMMA 5.7. *Let $\bar{q}_k \in Q_{ad}$ be the solution of the semidiscretized optimization problem* (3.4) *and $I_d\bar{q}_k$ be the interpolation constructed by* (5.5). *Then, if Assumption* 1 *is fulfilled, the following estimate holds for $n < p \le \infty$, provided $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$:*

$$\|I_d\bar{q}_k - \bar{q}_k\|_I \le \frac{C}{\alpha} \left\{ h^2 \|\nabla^2 z_k(\bar{q}_k)\|_I + h^{\frac{3}{2}-\frac{1}{p}} \|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))} \right\}.$$

Proof. Since $\bar{q}_k$ is piecewise constant in time we write

$$\|I_d\bar{q}_k - \bar{q}_k\|^2_I = \sum_{m=1}^{M} \int_{I_m} \|I_d\bar{q}_k(t) - \bar{q}_k(t)\|^2\, dt = \sum_{m=1}^{M} k_m \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2. \tag{5.10}$$

For each $m = 1, 2, \dots, M$, we split

$$\begin{aligned}\|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2 &= \sum_{K\in\mathcal{T}_h} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2_{L^2(K)} \\ &= \sum_{K\in\mathcal{T}^2_{h,m}} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2_{L^2(K)} \\ &\quad + \sum_{K\in\mathcal{T}^3_{h,m}} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2_{L^2(K)}.\end{aligned} \tag{5.11}$$

Here, the sum over $K \in \mathcal{T}^1_{h,m}$ vanishes since on $\mathcal{T}^1_{h,m}$ it holds that $I_d\bar{q}_k = \bar{q}_k$.

The first term on the right-hand side of (5.11) can be estimated as

$$\begin{aligned}\sum_{K\in\mathcal{T}^2_{h,m}} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2_{L^2(K)} &\le Ch^4 \sum_{K\in\mathcal{T}^2_{h,m}} \|\nabla^2\bar{q}_k(t_m)\|^2_{L^2(K)} \\ &\le \frac{C}{\alpha^2} h^4 \|\nabla^2 z_k(\bar{q}_k)(t_m)\|^2,\end{aligned}$$

since $\bar{q}_k(t_m) = -\frac{1}{\alpha} z_k(\bar{q}_k)(t_m)$ on all cells $K \in \mathcal{T}^2_{h,m}$. For the second term on the right-hand side of (5.11) we proceed by means of representation formula (3.9), property (2.10), and Assumption 1:

$$\begin{aligned}\sum_{K\in\mathcal{T}^3_{h,m}} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2_{L^2(K)} &\le \sum_{K\in\mathcal{T}^3_{h,m}} |K|^{1-\frac{2}{p}} \|I_d\bar{q}_k(t_m) - \bar{q}_k(t_m)\|^2_{L^p(K)} \\ &\le Ch^2 \sum_{K\in\mathcal{T}^3_{h,m}} |K|^{1-\frac{2}{p}} \|\nabla\bar{q}_k(t_m)\|^2_{L^p(K)} \\ &\le Ch^2 \left(\sum_{K\in\mathcal{T}^3_{h,m}} |K|\right)^{1-\frac{2}{p}} \|\nabla\bar{q}_k(t_m)\|^2_{L^p(\Omega)} \\ &\le \frac{C}{\alpha^2} h^{3-\frac{2}{p}} \|\nabla z_k(\bar{q}_k)(t_m)\|^2_{L^p(\Omega)}.\end{aligned}$$

Inserting the last two estimates into (5.11) and plugging (5.11) into (5.10) implies the stated result. ∎

Corollary 5.8. *Under the conditions of Theorem* 5.5 *and Lemmas* 5.6 *and* 5.7*, the following estimate holds:*

$$\begin{aligned}\|\bar{q} - \bar{q}_\sigma\|_I \le \frac{C}{\alpha} k\big\{\|\partial_t u(\bar{q})\|_I + \|\partial_t z(\bar{q})\|_I\big\} + \frac{C}{\alpha}\Big(1 + \frac{1}{\alpha}\Big)\big\{h^2\|\nabla^2 u_k(\bar{q}_k)\|_I \\ + h^2\|\nabla^2 z_k(\bar{q}_k)\|_I + h^{\frac{3}{2}-\frac{1}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))}\big\} = \mathcal{O}(k + h^{\frac{3}{2}-\frac{1}{p}}).\end{aligned}$$

Proof. The result follows directly from Theorems 5.1 and 5.5, Lemmas 5.6 and 5.7, and Proposition 4.4. ∎

In what follows we discuss the result from Corollary 5.8 in more details. This result holds under the assumption that $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$. From the stability result in Proposition 4.1 and the fact that $\bar{q}_k \in Q_{\text{ad}}$, we know that

$$\|z_k(\bar{q}_k)\|_{L^2(I,H^2(\Omega))} \le C.$$

By a Sobolev embedding theorem we have $H^2(\Omega) \hookrightarrow W^{1,p}(\Omega)$ for all $p < \infty$ in two space dimensions and for $p \leq 6$ in three dimensions. This implies the order of convergence $\mathcal{O}\big(k + h^{\frac{3}{2}-\frac{1}{p}}\big)$ for all $2 < p < \infty$ in two dimensions and $\mathcal{O}\big(k + h^{\frac{4}{3}}\big)$ in three dimensions, respectively. If in addition $\|z_k(\bar{q}_k)\|_{L^2(I,W^{1,\infty}(\Omega))}$ is bounded, then we have in both cases the order of convergence $\mathcal{O}\big(k + h^{\frac{3}{2}}\big)$.

Remark 5.9. The above result relies on Assumption 1. This assumption is valid in the majority of practical cases; cf. Remark 5.4. In the absence of this assumption a weaker result for the behavior of the spatial error can be shown, i.e.,

$$\lim_{h\to 0} \frac{1}{h} \|\bar{q}_k - \bar{q}_\sigma\|_I = 0.$$

The proofs in this section can simply be adapted to this situation. For the corresponding result for elliptic optimal control problems, we refer to [4].

5.3. Variational approach. In this subsection we prove an estimate for the error $\|\bar{q} - \bar{q}_\sigma\|_I$ in the case of no control discretization; see section 3.3.3. In this case we choose $Q_d = Q$, and thus $Q_{d,\mathrm{ad}} = Q_{\mathrm{ad}}$. This implies $\bar{q}_\sigma = \bar{q}_{kh}$.

THEOREM 5.10. *Let $\bar{q} \in Q_{ad}$ be the solution of optimization problem* (2.2) *and $\bar{q}_{kh} \in Q_{ad}$ be the solution of the discretized problem* (3.11). *Then the following estimate holds:*

$$\|\bar{q} - \bar{q}_{kh}\|_I \leq \frac{1}{\alpha} \|z(\bar{q}) - z_{kh}(\bar{q})\|_I.$$

Proof. The proof is similar to the proof of Theorem 5.1. The optimality conditions (2.4) and (3.12) lead to

$$-j'_{kh}(\bar{q}_{kh})(\bar{q} - \bar{q}_{kh}) \leq 0 \leq -j'(\bar{q})(\bar{q} - \bar{q}_{kh}).$$

Using (3.15) we have with any $p \in Q$,

$$\begin{aligned}
\alpha\|\bar{q} - \bar{q}_{kh}\|_I^2 &\leq j''_{kh}(p)(\bar{q} - \bar{q}_{kh}, \bar{q} - \bar{q}_{kh}) \\
&= j'_{kh}(\bar{q})(\bar{q} - \bar{q}_{kh}) - j'_{kh}(\bar{q}_{kh})(\bar{q} - \bar{q}_{kh}) \\
&\leq j'_{kh}(\bar{q})(\bar{q} - \bar{q}_{kh}) - j'(\bar{q})(\bar{q} - \bar{q}_{kh}) \\
&= (z(\bar{q}) - z_{kh}(\bar{q}), \bar{q} - \bar{q}_{kh})_I.
\end{aligned}$$

The desired assertion follows by Cauchy's inequality. ◻

This approach provides the optimal order of convergence stated in the following corollary.

COROLLARY 5.11. *Let the conditions of Theorem* 5.10 *be fulfilled. Then there holds*

$$\begin{aligned}
\|\bar{q} - \bar{q}_{kh}\|_I \leq \frac{C}{\alpha} k \big\{ \|\partial_t u(\bar{q})\|_I + \|\partial_t z(\bar{q})\|_I \big\} \\
+ \frac{C}{\alpha} h^2 \big\{ \|\nabla^2 u_k(\bar{q})\|_I + \|\nabla^2 z_k(\bar{q})\|_I \big\} = \mathcal{O}(k + h^2).
\end{aligned}$$

Proof. The proof follows directly from Theorem 5.10 and Propositions 4.3 and 4.4. ◻

5.4. Postprocessing strategy. In this section, we extend the postprocessing techniques initially proposed in [21] to the parabolic case. As described in section 3.3.4 we discretize the control by piecewise constants in time and space. To improve the quality of the approximation, we additionally employ the postprocessing step (3.18).

In what follows we will use the operator R_d defined for functions $g \in C(\bar{\Omega})$ cellwise by

$$R_d g\big|_K = g(S_K), \quad K \in \mathcal{T}_h,$$

where S_K denotes the barycenter of the cell K. This operator allows for the following interpolation estimates.

LEMMA 5.12. *Let $K \in \mathcal{T}_h$ be a given cell. Then we have that*

- *for $g \in H^2(K)$,*

$$\left| \int_K (g(x) - (R_d g)(x))\, dx \right| \le Ch^2 |K|^{\frac{1}{2}} \|\nabla^2 g\|_{L^2(K)};$$

- *for $g \in W^{1,p}(K)$ with $n < p \le \infty$,*

$$\|g - R_d g\|_{L^p(K)} \le Ch \|\nabla g\|_{L^p(K)}.$$

Proof. The proof is done by standard arguments using the Bramble–Hilbert lemma; see [21] for details. ◻

The operator R_d will also be used for time-dependent functions g by setting $(R_d g)(t) = R_d g(t)$. There holds the following lemma.

LEMMA 5.13. *For a function $g_k \in X_k^0 \cap L^2(I, H^2(\Omega))$ and a cellwise constant function $p_d \in Q_d$, the estimate*

$$(p_d, g_k - R_d g_k)_I \le Ch^2 \|p_d\|_I \|\nabla^2 g_k\|_I$$

holds.

Proof. Using Lemma 5.12 we obtain

$$\begin{aligned}
(p_d, g_k - R_d g_k)_I &= \sum_{m=1}^{M} \int_{I_m} (p_d(t), g_k(t) - R_d g_k(t))\, dt \\
&= \sum_{m=1}^{M} k_m (p_d(t_m), g_k(t_m) - R_d g_k(t_m)) \\
&= \sum_{m=1}^{M} k_m \sum_{K \in \mathcal{T}_h} p_d(t_m, S_K) \int_K (g_k(t_m, x) - (R_d g_k)(t_m, x))\, dx \\
&\le Ch^2 \sum_{m=1}^{M} k_m \sum_{K \in \mathcal{T}_h} |p_d(t_m, S_K)|\, |K|^{\frac{1}{2}} \|\nabla^2 g_k(t_m)\|_{L^2(K)}.
\end{aligned}$$

We complete the proof by Cauchy's inequality. ◻

LEMMA 5.14. *Let $\bar{q}_k \in Q_{ad}$ be the solution of the semidiscrete optimization problem* (3.4) *and $\bar{q}_\sigma \in Q_{d,ad}$ be the solution of the discrete problem* (3.16)*, where the cellwise constant control discretization is employed. Then the following relation holds:*

$$(\alpha R_d \bar{q}_k + R_d z_k(\bar{q}_k), \bar{q}_\sigma - R_d \bar{q}_k)_I \ge 0.$$

Proof. From the optimality condition (3.5) for $\bar{q}_k$, we obtain

$$(\alpha\bar{q}_k(t_m,x)+z_k(\bar{q}_k)(t_m,x))\cdot(\delta q(t_m,x)-\bar{q}_k(t_m,x))\geq 0$$

for any $\delta q\in Q_{d,\mathrm{ad}}$ pointwise a.e. in Ω and for $m=1,2,\ldots,M$. For an arbitrary cell $K\in\mathcal{T}_h$ we apply this formula for $x=S_K$ and $\delta q=\bar{q}_\sigma$:

$$(\alpha\bar{q}_k(t_m,S_K)+z_k(\bar{q}_k)(t_m,S_K))\cdot(\bar{q}_\sigma(t_m,S_K)-\bar{q}_k(t_m,S_K))\geq 0.$$

This can be done because of the spatial continuity of $z_k(\bar{q}_k)$, $\bar{q}_k$, and $\bar{q}_\sigma$. Due to the definition of R_d, this is equivalent to

$$(\alpha R_d\bar{q}_k(t_m,S_K)+R_d z_k(\bar{q}_k)(t_m,S_K))\cdot(\bar{q}_\sigma(t_m,S_K)-R_d\bar{q}_k(t_m,S_K))\geq 0.$$

Then, integration over K and I_m, summation over all $K\in\mathcal{T}_h$, and $m=1,2,\ldots,M$ lead to the proposed relation. ▯

LEMMA 5.15. *Let $\bar{q}_k\in Q_{ad}$ be the solution of the semidiscrete optimization problem* (3.4) *and let $\psi_{kh}\in X^{0,1}_{k,h}$. Moreover, let Assumption* 1 *be fulfilled and $n<p\leq\infty$. Then, it holds that*

$$(\psi_{kh},\bar{q}_k-R_d\bar{q}_k)_I\leq\frac{C}{\alpha}h^2\big\{\|\nabla\psi_{kh}\|_I\|\nabla z_k(\bar{q}_k)\|_I+\|\psi_{kh}\|_{L^2(I,L^\infty(\Omega))}\|\nabla^2 z_k(\bar{q}_k)\|_I\big\}$$
$$+\frac{C}{\alpha}h^{2-\frac{1}{p}}\|\psi_{kh}\|_{L^2(I,L^\infty(\Omega))}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))},$$

provided that $z_k(\bar{q}_k)\in L^2(I,W^{1,p}(\Omega))$.

Proof. By means of the L^2-projection $\pi_d\colon Q\to Q_d$, we split

$$(\psi_{kh},\bar{q}_k-R_d\bar{q}_k)_I=(\psi_{kh},\bar{q}_k-\pi_d\bar{q}_k)_I+(\psi_{kh},\pi_d\bar{q}_k-R_d\bar{q}_k)_I.$$

Using the optimality condition (3.9) and property (2.10) of the projection operator $P_{Q_{\mathrm{ad}}}$, we have for the first term

$$\begin{aligned}(\psi_{kh},\bar{q}_k-\pi_d\bar{q}_k)_I&=(\psi_{kh}-\pi_d\psi_{kh},\bar{q}_k-\pi_d\bar{q}_k)_I\leq Ch^2\|\nabla\psi_{kh}\|_I\|\nabla\bar{q}_k\|_I\\&\leq\frac{C}{\alpha}h^2\|\nabla\psi_{kh}\|_I\|\nabla z_k(\bar{q}_k)\|_I.\end{aligned}\tag{5.12}$$

For the second term we obtain

$$\begin{aligned}(\psi_{kh},\pi_d\bar{q}_k-R_d\bar{q}_k)_I&=\sum_{m=1}^M\int_{I_m}(\psi_{kh}(t),\pi_d\bar{q}_k(t)-R_d\bar{q}_k(t))\,dt\\&=\sum_{m=1}^M k_m(\psi_{kh}(t_m),\pi_d\bar{q}_k(t_m)-R_d\bar{q}_k(t_m)).\end{aligned}$$

Utilizing the fact that $\pi_d\bar{q}_k(t_m)$ as well as $R_d\bar{q}_k(t_m)$ are constant on each cell K, we proceed with

$$
\begin{aligned}
&(\psi_{kh}(t_m), \pi_d \bar{q}_k(t_m) - R_d \bar{q}_k(t_m)) \\
&\quad = \sum_{K \in \mathcal{T}_h} \int_K \psi_{kh}(t_m, x)(\pi_d \bar{q}_k(t_m, x) - (R_d \bar{q}_k)(t_m, x))\, dx \\
&\quad = \sum_{K \in \mathcal{T}_h} \frac{1}{|K|} \int_K \psi_{kh}(t_m, x)\, dx \int_K (\pi_d \bar{q}_k(t_m, x) - (R_d \bar{q}_k)(t_m, x))\, dx \\
&\quad \le \|\psi_{kh}(t_m)\|_{L^\infty(\Omega)} \sum_{K \in \mathcal{T}_h} \left| \int_K (\bar{q}_k(t_m, x) - (R_d \bar{q}_k)(t_m, x))\, dx \right|.
\end{aligned}
\tag{5.13}
$$

As in section 5.2, we split the last sum using the separation $\mathcal{T}_h = \mathcal{T}_{h,m}^1 \cup \mathcal{T}_{h,m}^2 \cup \mathcal{T}_{h,m}^3$ for $m = 1, 2, \ldots, M$. For the sum over $\mathcal{T}_{h,m}^1 \cup \mathcal{T}_{h,m}^2$ we obtain by means of Lemma 5.12 and the fact that $\bar{q}_k(t_m)$ equals either q_a, q_b, or $-\frac{1}{\alpha} z_k(\bar{q}_k)(t_m)$:

$$
\begin{aligned}
&\sum_{K \in \mathcal{T}_{h,m}^1 \cup \mathcal{T}_{h,m}^2} \left| \int_K (\bar{q}_k(t_m, x) - R_d \bar{q}_k(t_m, x))\, dx \right| \\
&\qquad \le C h^2 \sum_{K \in \mathcal{T}_{h,m}^1 \cup \mathcal{T}_{h,m}^2} |K|^{\frac{1}{2}} \|\nabla^2 \bar{q}_k(t_m)\|_{L^2(K)} \\
&\qquad \le \frac{C}{\alpha} h^2 \|\nabla^2 z_k(\bar{q}_k)(t_m)\|.
\end{aligned}
\tag{5.14}
$$

For the part of the sum over $\mathcal{T}_{h,m}^3$, the estimate of Lemma 5.12, Assumption 1, the optimality condition (3.9), and property (2.10) lead to

$$
\begin{aligned}
\sum_{K \in \mathcal{T}_{h,m}^3} \left| \int_K (\bar{q}_k(t_m, x) - R_d \bar{q}_k(t_m, x))\, dx \right| &\le \sum_{K \in \mathcal{T}_{h,m}^3} |K|^{1-\frac{1}{p}} \|\bar{q}_k(t_m) - R_d \bar{q}_k(t_m)\|_{L^p(K)} \\
&\le C h \sum_{K \in \mathcal{T}_{h,m}^3} |K|^{1-\frac{1}{p}} \|\nabla \bar{q}_k(t_m)\|_{L^p(K)} \\
&\le \frac{C}{\alpha} h^{2-\frac{1}{p}} \|\nabla z_k(\bar{q}_k(t_m))\|_{L^p(\Omega)}.
\end{aligned}
\tag{5.15}
$$

Inserting (5.14) and (5.15) into (5.13) and collecting the estimates (5.12) and (5.13) completes the proof. □

The following theorem provides a supercloseness result on the difference $R_d \bar{q}_k - \bar{q}_\sigma$.

THEOREM 5.16. *Let $\bar{q}_k \in Q_{ad}$ be the solution of the semidiscretized optimization problem* (3.4) *and $\bar{q}_\sigma \in Q_{d,ad}$ be the solution of the discrete problem* (3.16)*, where the cellwise constant discretization for the control variable is employed. Moreover, let*

Assumption 1 *be fulfilled and* $n < p \leq \infty$. *Then, it holds that*

$$\|R_d\bar{q}_k - \bar{q}_\sigma\|_I \leq \frac{C}{\alpha}h^2 \left\{ \|\nabla^2 u_k(\bar{q}_k)\|_I + \frac{1}{\alpha}\|\nabla z_k(\bar{q}_k)\|_I + \left(1+\frac{1}{\alpha}\right)\|\nabla^2 z_k(\bar{q}_k)\|_I \right\} + \frac{C}{\alpha^2}h^{2-\frac{1}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))},$$

provided that $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$.

Proof. As before, we proceed with an arbitrary $p \in Q$,

$$\begin{aligned} \alpha\|R_d\bar{q}_k - \bar{q}_\sigma\|_I^2 &\leq j''_{kh}(p)(R_d\bar{q}_k - \bar{q}_\sigma, R_d\bar{q}_k - \bar{q}_\sigma) \\ &= j'_{kh}(R_d\bar{q}_k)(R_d\bar{q}_k - \bar{q}_\sigma) - j'_{kh}(\bar{q}_\sigma)(R_d\bar{q}_k - \bar{q}_\sigma). \end{aligned}$$

By means of the inequality

$$-j'_{kh}(\bar{q}_\sigma)(R_d\bar{q}_k - \bar{q}_\sigma) \leq 0 \leq -(\alpha R_d\bar{q}_k + R_d z_k(\bar{q}_k), R_d\bar{q}_k - \bar{q}_\sigma)_I,$$

which is implied by the optimality of $\bar{q}_\sigma$ and Lemma 5.14, and by means of the explicit representation of j'_{kh} from (3.13), we obtain

$$\begin{aligned} \alpha\|R_d\bar{q}_k - \bar{q}_\sigma\|_I^2 &\leq (z_{kh}(R_d\bar{q}_k) - R_d z_k(\bar{q}_k), R_d\bar{q}_k - \bar{q}_\sigma)_I \\ &\leq (z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k), R_d\bar{q}_k - \bar{q}_\sigma)_I \\ &\quad + (z_k(\bar{q}_k) - R_d z_k(\bar{q}_k), R_d\bar{q}_k - \bar{q}_\sigma)_I. \end{aligned} \tag{5.16}$$

For the first term on the right-hand side of (5.16), we have by Cauchy's inequality,

$$(z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k), R_d\bar{q}_k - \bar{q}_\sigma)_I \leq \|z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k)\|_I \|R_d\bar{q}_k - \bar{q}_\sigma\|_I.$$

By insertion of $z_{kh}(\bar{q}_k)$, the term $\|z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k)\|_I$ is further estimated as

$$\|z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k)\|_I \leq \|z_{kh}(R_d\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I + \|z_{kh}(\bar{q}_k) - z_k(\bar{q}_k)\|_I. \tag{5.17}$$

Due to the stability estimate of the fully discrete adjoint solution (see Proposition 4.2), the first term is bounded by

$$\|z_{kh}(R_d\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I \leq C\|u_{kh}(R_d\bar{q}_k) - u_{kh}(\bar{q}_k)\|_I. \tag{5.18}$$

Further, we have by means of the discrete state equation (3.10) and the discrete adjoint equation (3.14),

$$\|u_{kh}(R_d\bar{q}_k) - u_{kh}(\bar{q}_k)\|_I^2 = (z_{kh}(\bar{q}_k) - z_{kh}(R_d\bar{q}_k), \bar{q}_k - R_d\bar{q}_k)_I.$$

With $\psi_{kh} = z_{kh}(\bar{q}_k) - z_{kh}(R_d\bar{q}_k)$ in Lemma 5.15, we have

$$\begin{aligned} \|u_{kh}(R_d\bar{q}_k) - u_{kh}(\bar{q}_k)\|_I^2 \leq \frac{C}{\alpha}h^2 \big\{ &\|\nabla(z_{kh}(\bar{q}_k) - z_{kh}(R_d\bar{q}_k))\|_I \|\nabla z_k(\bar{q}_k)\|_I \\ &+ \|z_{kh}(\bar{q}_k) - z_{kh}(R_d\bar{q}_k)\|_{L^2(I,L^\infty(\Omega))} \|\nabla^2 z_k(\bar{q}_k)\|_I \big\} \\ + \frac{C}{\alpha}h^{2-\frac{1}{p}} &\|z_{kh}(\bar{q}_k) - z_{kh}(R_d\bar{q}_k)\|_{L^2(I,L^\infty(\Omega))} \|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))}, \end{aligned}$$

and the stability estimates from Proposition 4.2 and Lemma 4.5,

$$\|\nabla(z_{kh}(q_k) - z_{kh}(R_d q_k))\|_I \leq C\|u_{kh}(R_d q_k) - u_{kh}(q_k)\|_I,$$
$$\|z_{kh}(q_k) - z_{kh}(R_d q_k)\|_{L^2(I,L^\infty(\Omega))} \leq C\|u_{kh}(R_d q_k) - u_{kh}(q_k)\|_I,$$

yield the following intermediary result:

$$\|u_{kh}(R_d\bar{q}_k) - u_{kh}(\bar{q}_k)\|_I \leq \frac{C}{\alpha}h^2\big\{\|\nabla z_k(\bar{q}_k)\|_I + \|\nabla^2 z_k(\bar{q}_k)\|_I\big\} + \frac{C}{\alpha}h^{2-\frac{1}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))}.$$

We proceed by inserting this in (5.18) and in (5.17). Together with an estimate for the second term on the right-hand side of (5.17) from Proposition 4.4, this leads to

$$\|z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k)\|_I \leq Ch^2\left\{\|\nabla^2 u_k(\bar{q}_k)\|_I + \frac{1}{\alpha}\|\nabla z_k(\bar{q}_k)\|_I + \Big(1+\frac{1}{\alpha}\Big)\|\nabla^2 z_k(\bar{q}_k)\|_I\right\} + \frac{C}{\alpha}h^{2-\frac{1}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))}. \tag{5.19}$$

By applying Lemma 5.13 with $p_d = R_d\bar{q}_k - \bar{q}_\sigma$ to the second term on the right-hand side of (5.16), we get

$$(z_k(\bar{q}_k) - R_d z_k(\bar{q}_k), R_d\bar{q}_k - \bar{q}_\sigma)_I \leq Ch^2\|R_d\bar{q}_k - \bar{q}_\sigma\|_I\|\nabla^2 z_k(\bar{q}_k)\|_I.$$

The asserted result is obtained by insertion of the last two estimates into (5.16). ◻

Based on this theorem, we state the main result of this section concerning the order of convergence of the error between $\bar{q}$ and $\tilde{q}_\sigma$, where $\tilde{q}_\sigma$ is defined using the postprocessing step (3.18).

Corollary 5.17. *Let the conditions of Theorem* 5.16 *be fulfilled. Then, there holds*

$$\begin{aligned}\|\bar{q} - \tilde{q}_\sigma\|_I &\leq \frac{C}{\alpha}\Big(1+\frac{1}{\alpha}\Big)k\big\{\|\partial_t u(\bar{q})\|_I + \|\partial_t z(\bar{q})\|_I\big\}\\ &+ \frac{C}{\alpha}\Big(1+\frac{1}{\alpha}\Big)h^2\left\{\|\nabla^2 u_k(\bar{q}_k)\|_I + \frac{1}{\alpha}\|\nabla z_k(\bar{q}_k)\|_I + \Big(1+\frac{1}{\alpha}\Big)\|\nabla^2 z_k(\bar{q}_k)\|_I\right\}\\ &+ \frac{C}{\alpha^2}\Big(1+\frac{1}{\alpha}\Big)h^{2-\frac{1}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))} = \mathcal{O}\big(k + h^{2-\frac{1}{p}}\big).\end{aligned}$$

Proof. From the optimality condition (2.9) and the definition (3.18) of $\tilde{q}_\sigma$ we have the representation

$$\|\bar{q} - \tilde{q}_\sigma\|_I = \left\|P_{Q_{\mathrm{ad}}}\left(-\frac{1}{\alpha}z(\bar{q})\right) - P_{Q_{\mathrm{ad}}}\left(-\frac{1}{\alpha}z_{kh}(\bar{q}_\sigma)\right)\right\|_I.$$

By means of the Lipschitz continuity of $P_{Q_{\mathrm{ad}}}$ on $L^2(I, L^2(\Omega))$, this leads to

$$\alpha\|\bar{q} - \tilde{q}_\sigma\|_I \leq \|z(\bar{q}) - z_{kh}(\bar{q}_\sigma)\|_I \leq \|z(\bar{q}) - z_k(\bar{q}_k)\|_I + \|z_k(\bar{q}_k) - z_{kh}(\bar{q}_\sigma)\|_I. \tag{5.20}$$

The first term is controlled by means of Proposition 4.1, Theorem 5.1, and Proposition 4.3 as

$$\begin{aligned}\|z(\bar{q}) - z_k(\bar{q}_k)\|_I &\le \|z(\bar{q}) - z_k(\bar{q})\|_I + \|z_k(\bar{q}) - z_k(\bar{q}_k)\|_I \\ &\le \|z(\bar{q}) - z_k(\bar{q})\|_I + C\|u_k(\bar{q}) - u_k(\bar{q}_k)\|_I \\ &\le \|z(\bar{q}) - z_k(\bar{q})\|_I + C\|\bar{q} - \bar{q}_k\|_I \\ &\le \Big(1 + \frac{C}{\alpha}\Big)\|z(\bar{q}) - z_k(\bar{q})\|_I \\ &\le C\Big(1 + \frac{1}{\alpha}\Big)k\big\{\|\partial_t u(\bar{q})\|_I + \|\partial_t z(\bar{q})\|_I\big\}.\end{aligned}$$

The second term can be estimated by means of the stability result of Proposition 4.2 as

$$\begin{aligned}\|z_k(\bar{q}_k) - z_{kh}(\bar{q}_\sigma)\|_I &\le \|z_k(\bar{q}_k) - z_{kh}(R_d\bar{q}_k)\|_I + \|z_{kh}(R_d\bar{q}_k) - z_{kh}(\bar{q}_\sigma)\|_I \\ &\le \|z_k(\bar{q}_k) - z_{kh}(R_d\bar{q}_k)\|_I + C\|u_{kh}(R_d\bar{q}_k) - u_{kh}(\bar{q}_\sigma)\|_I \\ &\le \|z_k(\bar{q}_k) - z_{kh}(R_d\bar{q}_k)\|_I + C\|R_d\bar{q}_k - \bar{q}_\sigma\|_I.\end{aligned}$$

Inserting the two last inequalities into (5.20) and applying the estimates from (5.19) and Theorem 5.16 yield the stated assertion. ∎

The choice of p in Corollary 5.17 follows the description in section 5.2 requiring $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$. Due to the fact that $\|z_k(\bar{q}_k)\|_{L^2(I,H^2(\Omega))}$ is bounded independently of k, the result in Corollary 5.17 holds for any $n < p < \infty$ in the two dimensional case, leading to the order of convergence $\mathcal{O}\big(k + h^{2-\frac{1}{p}}\big)$. In the three dimensional case we obtain $p = 6$ and therefore $\mathcal{O}\big(k + h^{\frac{11}{6}}\big)$. If in addition $\|z_k(\bar{q}_k)\|_{L^2(I,W^{1,\infty}(\Omega))}$ is bounded, then we have in both cases the order of convergence $\mathcal{O}(k + h^2)$.

6. Numerical results.

In this section, we are going to validate the a priori error estimates for the error in the control, state, and adjoint state numerically. To this end, we consider the following concretion of the optimal control problem (2.2) with known exact solution on $\Omega \times I = (0,1)^2 \times (0, 0.1)$ and homogeneous Dirichlet boundary conditions. According to the first part of this article [20], the right-hand side f, the desired state $\hat{u}$, and the initial condition u_0 are given in terms of the eigenfunctions

$$w_a(t, x_1, x_2) \coloneqq \exp(a\pi^2 t)\sin(\pi x_1)\sin(\pi x_2), \quad a \in \mathbb{R},$$

of the operator $\pm\partial_t - \Delta$ as

$$\begin{aligned}f(t, x_1, x_2) &\coloneqq -\pi^4 w_a(t, x_1, x_2) - P_{Q_{\mathrm{ad}}}\big(-\pi^4\{w_a(t, x_1, x_2) - w_a(T, x_1, x_2)\}\big), \\ \hat{u}(t, x_1, x_2) &\coloneqq \frac{a^2 - 5}{2 + a}\pi^2 w_a(t, x_1, x_2) + 2\pi^2 w_a(T, x_1, x_2), \\ u_0(x_1, x_2) &\coloneqq \frac{-1}{2 + a}\pi^2 w_a(0, x_1, x_2),\end{aligned}$$

with $P_{Q_{\mathrm{ad}}}$ given by (2.8) with $q_a = -70$ and $q_b = -1$. For this choice of data and with the regularization parameter α chosen as $\alpha = \pi^{-4}$, the optimal solution triple

$(\bar{q}, \bar{u}, \bar{z})$ of the optimal control problem (2.2) is given by

$$\bar{q}(t, x_1, x_2) := P_{Q_{\mathrm{ad}}}\big(-\pi^4\{w_a(t, x_1, x_2) - w_a(T, x_1, x_2)\}\big),$$

$$\bar{u}(t, x_1, x_2) := \frac{-1}{2+a}\pi^2 w_a(t, x_1, x_2),$$

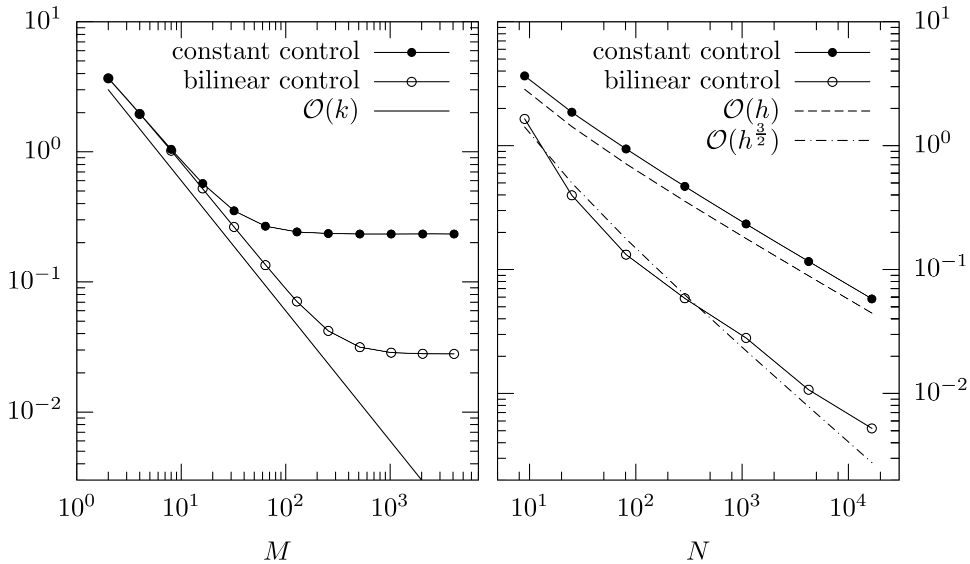
$$\bar{z}(t, x_1, x_2) := w_a(t, x_1, x_2) - w_a(T, x_1, x_2).$$

We are going to validate the estimates developed in the previous section by separating the discretization errors. That is, we consider at first the behavior of the error for a sequence of discretizations with decreasing size of the time steps and a fixed spatial triangulation with $N = 1089$ nodes. Second, we examine the behavior of the error under refinement of the spatial triangulation for $M = 2048$ time steps.

The state discretization is chosen as cG(1)dG(0), i.e., $r = 0$, $s = 1$. For the control discretization we use the same temporal and spatial meshes as for the state variable and present results for two choices of the discrete control space Q_d: cG(1)dG(0) and dG(0)dG(0). For the following computations, we choose the free parameter a to be $-\sqrt{5}$.

The optimal control problems are solved by the optimization library RoDoBo [22] and the finite element toolkit Gascoigne [11] using a primal-dual active set strategy (cf. [3, 14]) in combination with a conjugate gradient method applied to the reduced problem (3.16).

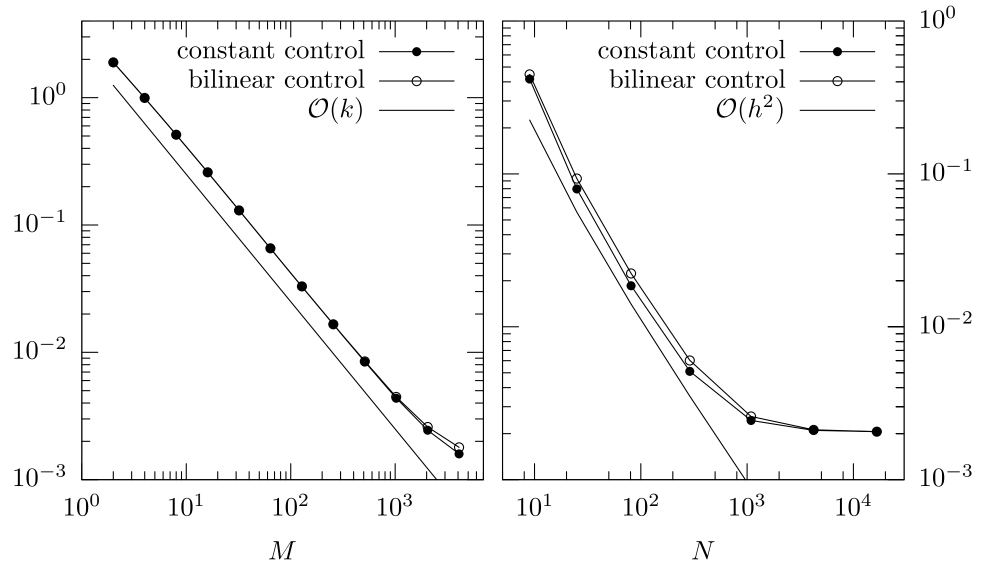
Figure 6.1(a) depicts the development of the error under refinement of the temporal step size k. Up to the spatial discretization error it exhibits the proven convergence order $\mathcal{O}(k)$ for both kinds of spatial discretization of the control space.



(a) Refinement of the time steps for $N = 1089$ spatial nodes.

(b) Refinement of the spatial triangulation for $M = 2048$ time steps.

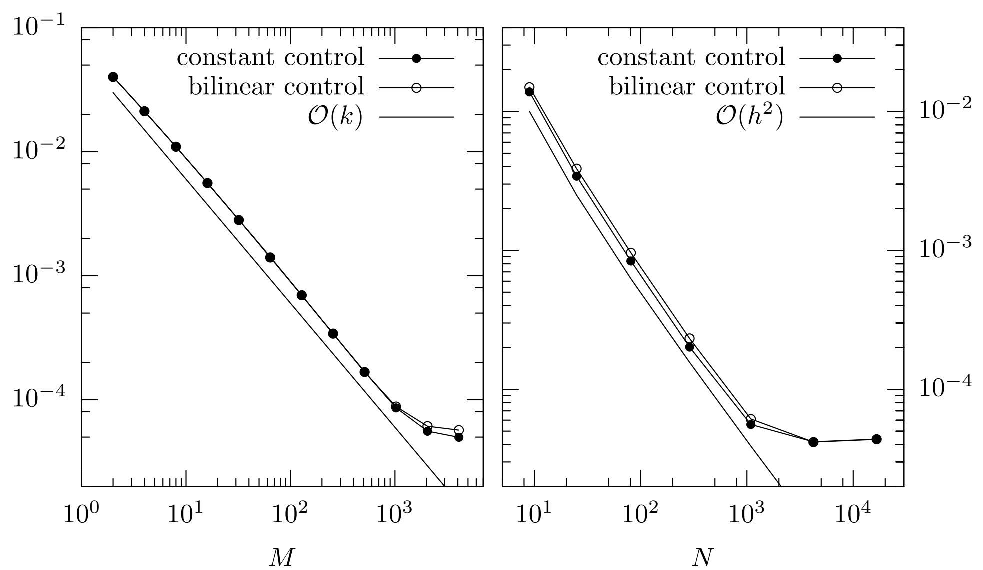
Fig. 6.1. *Discretization error* $\|\bar{q} - \bar{q}_\sigma\|_I$.



(a) Refinement of the time steps for $N = 1089$ spatial nodes.

(b) Refinement of the spatial triangulation for $M = 2048$ time steps.

FIG. 6.2. *Discretization error* $\|\bar{u} - \bar{u}_\sigma\|_I$.



(a) Refinement of the time steps for $N = 1089$ spatial nodes.

(b) Refinement of the spatial triangulation for $M = 2048$ time steps.

FIG. 6.3. *Discretization error* $\|\bar{z} - \bar{z}_\sigma\|_I$.

For piecewise constant control (dG(0)dG(0) discretization), the discretization error is already reached at 128 time steps, whereas in the case of bilinear control (cG(1)dG(0) discretization), the number of time steps could be increased up to $M = 1024$ until reaching the spatial accuracy. This illustrates the convergence results from sections 5.1 and 5.2 with respect to the *temporal* discretization.

In Figure 6.1(b) the development of the error in the control variable under spatial refinement is shown. The expected order $\mathcal{O}(h)$ for piecewise constant control (dG(0)dG(0) discretization) and $\mathcal{O}(h^{\frac{3}{2}})$ for bilinear control (cG(1)dG(0) discretization) are observed. This illustrates the convergence results from sections 5.1 and 5.2 with respect to the *spatial* discretization.

Figures 6.2 and 6.3 show the errors in the state and in the adjoint variables, $\|\bar{u} - \bar{u}_\sigma\|_I$ and $\|\bar{z} - \bar{z}_\sigma\|_I$, for separate refinement of the time and space discretization. Thereby, we observe convergence of order $\mathcal{O}(k + h^2)$ regardless of the type of spatial discretization used for the controls. This is consistent with the results proved in the previous section. Since the postprocessing strategy presented in section 5.4 relies essentially on the convergence properties of the adjoint variable, Figure 6.3 confirms the proven order of convergence of the error $\|\bar{q} - \tilde{q}_\sigma\|_I$.

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