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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

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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

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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 [18] 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.

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:

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

subject to

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

and

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

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.

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., [8, 10, 1, 11, 19, 5], there are only few published results on this topic for parabolic problems, see [17, 26, 14, 16, 21].

In the first part of our work on a priori error analysis of parabolic optimal control problems [18], we developed a priori error estimates for problems without control

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constrains. 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 [18].

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 [13].

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 the 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 [8, 10], the convergence order $\mathcal{O}(h)$ was established using a cellwise constant discretization of the control variable; see also [6, 1, 5]. 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., [4, 22, 2]. Recently, two approaches achieving $\mathcal{O}(h^2)$-convergence for the error in the control variable have been established; see [11, 19]. In [11] 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 [19] a cellwise constant discretization is utilized, and a *post-processing step* is used to obtain the desired accuracy. The later technique is extended to optimal control of the Stokes equations in [23].

For discretization of parabolic problems 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. [18].

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 [14, 16] the order of convergence $\mathcal{O}(h + k)$: The result is obtained under weaker regularity assumptions than in [14, 16]. 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 5.7. 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 proven 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 [11], 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 5.9. The usage of this approach requires a non-standard 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 post-processing strategy extending the technique from [19] 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 post-processing 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 5.15. 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), 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 discretization 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 before. In Section 4 we provide basic results on stability and approximation quality proved in the first part of this article [18]. 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

$$X \coloneqq \left\{\, v \;\middle|\; v \in L^2(I, V) \text{ and } \partial_t v \in L^2(I, V^*) \,\right\}$$

and the control space

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

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

$$\begin{aligned} (v, w) &\coloneqq (v, w)_{L^2(\Omega)}, & \qquad (v, w)_I &\coloneqq (v, w)_{L^2(I, L^2(\Omega))}, \\ \|v\| &\coloneqq \|v\|_{L^2(\Omega)}, & \qquad \|v\|_I &\coloneqq \|v\|_{L^2(I, L^2(\Omega))}. \end{aligned}$$

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: 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 [18], we use the following result on existence and regularity:

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*

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

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

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

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

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

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 [15].

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 $j \colon Q \to \mathbb{R}$:

$$j(q) \coloneqq J(q, u(q)).$$

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

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

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

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

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

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

Employing this formulation 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 the continuity of $P_{Q_{\mathrm{ad}}} \colon W^{1,p}(\Omega) \to W^{1,p}(\Omega)$ implies the desired result for $\bar{q}$. $\square$

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 the lines of the first part of this article [18]. 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

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

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 notations

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

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 $B(\cdot,\cdot)$ 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) semi-discretization of the state equation (2.1) for given control $q \in Q$ reads: 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 [25] 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 $r = 0$. This is reasonable due to the limited regularity caused by pointwise control constraints. 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:

$$\begin{aligned}
(U_1,\psi) + k_1(\nabla U_1,\nabla\psi) &= (f+q,\psi)_{I_m} + (u_0,\psi) && \forall \psi \in V,\\
(U_m,\psi) + k_m(\nabla U_m,\nabla\psi) &= (f+q,\psi)_{I_m} + (U_{m-1},\psi) && \forall \psi \in V,\ m = 2,3,\dots,M.
\end{aligned}$$

The semi-discrete optimization problem for the dG(0) time discretization has the 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 [18] the following result holds:

Proposition 3.1. *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.

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

$$j_k(q) \coloneqq J(q, u_k(q))$$

and reformulate the semidiscrete optimal control problem (3.4) as

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

The first order necessary optimality condition reads as

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

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.

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

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

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

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., [7]. 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:

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

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. [18].

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

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

Remark 3.2. *Here, the spatial mesh and therefore also the space V_h^s is fixed for all time intervals. We refer to [24] 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 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

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

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

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

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

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

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

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

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

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

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

The unique optimal solution of (3.16) is denoted by $(\bar{q}_\sigma, \bar{u}_\sigma) \in Q_{d,\mathrm{ad}} \times X_{k,h}^{0,1}$, 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:

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

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 the same spatial mesh as for the discretization of the state variable we set

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

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 control discretization as for the state variable, i.e. piecewise constant in time and cellwise (bi-/tri-)linear in space. Using a spatial space

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

we set

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

The state space $X^{0,1}_{k,h}$ coincides with the control space Q_d in case of homogeneous Neumann boundary conditions and is a subspace of it, i.e., $Q_d \supset X^{0,1}_{k,h}$ 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 [11], we can choose $Q_d = Q$. In this case the optimization problems (3.11) and (3.16) coincide and therefore, $\bar{q}_\sigma = \bar{q}_{kh} \in Q_{\mathrm{ad}}$.

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

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

and obtain that $\bar{q}_{kh}$ is 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 $\bar{q}_{kh}$, see [11] for details.

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

3.3.4. Post-processing strategy. The strategy described in this section extends the approach from [19] 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 post-processing 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 variational approach in Section 3.3.3, the solution $\tilde{q}_\sigma$ is piecewise constant in time and is general 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 [18], which will be used in the sequel.

The first proposition provides a stability result for the purely time discretized state and adjoint solutions. It follows from an estimate in [18] and elliptic regularity.

PROPOSITION 4.1. *Let for $q \in Q$ 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*

$$\begin{aligned}\|\nabla^2 u_k(q)\|_I + \|\nabla u_k(q)\|_I + \|u_k(q)\|_I &\le C\big\{\|f+q\|_I + \|\nabla u_0\| + \|u_0\|\big\},\\ \|\nabla^2 z_k(q)\|_I + \|\nabla z_k(q)\|_I + \|z_k(q)\|_I &\le C\|u_k(q) - \hat{u}\|_I.\end{aligned}$$

A similar result holds for the fully discretized solutions of the state and adjoint equations:

PROPOSITION 4.2. *Let for $q \in Q$ 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*

$$\begin{aligned}\|\nabla u_{kh}(q)\|_I + \|u_{kh}(q)\|_I &\le C\big\{\|f+q\|_I + \|\nabla \Pi_h u_0\| + \|\Pi_h u_0\|\big\},\\ \|\nabla z_{kh}(q)\|_I + \|z_{kh}(q)\|_I &\le C\|u_{kh}(q) - \hat{u}\|_I,\end{aligned}$$

where $\Pi_h \colon V \to V_h$ denotes the spacial 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:

PROPOSITION 4.3. *Let for $q \in Q$ 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 holds:*

$$\begin{aligned}\|u(q) - u_k(q)\|_I &\le Ck\|\partial_t u(q)\|_I,\\ \|z(q) - z_k(q)\|_I &\le Ck\big\{\|\partial_t u(q)\|_I + \|\partial_t z_k(q)\|_I\big\}.\end{aligned}$$

PROPOSITION 4.4. *Let for $q \in Q$ 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 $u_{kh}(q) \in X_{k,h}^{0,1}$ and $z_{kh}(q) \in X_{k,h}^{0,1}$ be determined as solutions of the discrete state equation* (3.10) *and adjoint equation* (3.14)*. Then the following error estimates holds:*

$$\begin{aligned}\|u_k(q) - u_{kh}(q)\|_I &\le Ch^2\|\nabla^2 u_k(q)\|_I,\\ \|z_k(q) - z_{kh}(q)\|_I &\le Ch^2\big\{\|\nabla^2 u_k(q)\|_I + \|\nabla^2 z_k(q)\|_I\big\}.\end{aligned}$$

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. *Let for $q \in Q$ 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*

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

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

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

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 $L^2(I, L^\infty(\Omega)) \hookrightarrow L^2(I, H^2(\Omega))$ we get

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

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

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

For the first term on the right-hand side of (4.1) we proceed by means of an inverse estimate, an estimate for the error due to space discretization (cf. [18]), and an interpolation estimate as

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

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

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

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

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

□

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:*

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

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

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

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

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

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

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

The desired assertion follows by Cauchy's inequality. ∎

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 [6] to the case of parabolic optimal control problems. This demands the introduction of the solution $\bar{q}_d$ of the purely control discretized problem

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

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

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

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:

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

THEOREM 5.2. *Let $\bar{q} \in Q_{ad}$ be the solution of the optimal control problem* (2.3), *$\bar{q}_\sigma \in Q_{d,ad}$ be the solution of the discretized problem* (3.16), *where the cellwise constant discretization for the control variable is employed. Let moreover $\bar{q}_d \in Q_{d,ad}$ 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

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

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

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

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

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

and by Young's inequality we obtain the intermediary result

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

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:

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

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:*

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

Proof. The assertion follows from Theorem 5.2 by interpolation estimates and the Propositions 4.3 and 4.4. Due to the fact $\bar{q}, \bar{q}_d \in Q_d$, we obtain using stability estimates 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

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

and use the result of Theorem 5.1 for the first part. For treating the error $\|\bar{q}_k - \bar{q}_\sigma\|$ we adapt the technique described in [2] 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 of the mesh $\mathcal{T}_h$ into two classes $\mathcal{T}_h = \mathcal{T}_{h,m}^1 \cup \mathcal{T}_{h,m}^2$ with $\mathcal{T}_{h,m}^1 \cap \mathcal{T}_{h,m}^2 = \emptyset$ as follows: The cell K belongs to $\mathcal{T}_{h,m}^1$ if and only if one of the following conditions is satisfied:

(a) $\bar{q}_k = q_a$ on $I_m \times K$,
(b) $\bar{q}_k = q_b$ on $I_m \times K$,
(c) $q_a < \bar{q}_k < q_b$ on $I_m \times K$.

The set $\mathcal{T}_{h,m}^2$ is given by $\mathcal{T}_{h,m}^2 = \mathcal{T}_h \setminus \mathcal{T}_{h,m}^1$ and consists of the cells which lie "close to 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*

$$\sum_{K \in \mathcal{T}_{h,m}^2} |K| \leq Ch.$$

Remark 5.1. *A similar assumption is used in [19, 23, 2]. This assumption is valid if the boundary of the level sets*

$$\{\, x \mid \bar{q}_k(t_m, x) = q_a \,\} \quad \textit{and} \quad \{\, x \mid \bar{q}_k(t_m, x) = q_b \,\}$$

consists of a finite number of rectifiable curves.

In what follows we will exploit a special interpolation $I_h \bar{q}_k \in Q_d$ of $\bar{q}_k$ which is defined using the information on the active sets of $\bar{q}_k$. To this end we introduce the patch $\omega(x_i)$ for each node x_i in $\mathcal{T}_h$ consisting of all cells K with $x_i \in \partial K$. Then the interpolant $I_h \bar{q}_k \in Q_d$ is given piecewise for $t \in I_m$ $(m = 1, 2, \ldots, M)$ by

$$I_h \bar{q}_k(t, x_i) = \begin{cases} q_a, & \text{if } \min\limits_{x \in \bar{\omega}(x_i)} \bar{q}_k(t_m, x) = q_a, \\ q_b, & \text{if } \max\limits_{x \in \bar{\omega}(x_i)} \bar{q}_k(t_m, x) = q_b, \\ \bar{q}_k(t_m, x_i), & \text{otherwise.} \end{cases} \tag{5.5}$$

A similar construction can be found in [6, 2].

In order to ensure that this interpolation is well-defined, one has to check that the first and second cases in (5.5) can not apply for the same node x_i. This requires an assumption on the smallness of the discretization parameter h:

Lemma 5.4. *Let a positive constant γ be chosen arbitrarily with $\gamma < 1$ for $n = 2$ and $\gamma < \frac{1}{2}$ for $n = 3$. Then, there exists a positive constant C independent of discretization parameters k, h and of the regularization parameter α such that the condition*

$$Ch^\gamma \leq \alpha k_m^{\frac{1}{2}} (q_b - q_a)$$

is sufficient to ensure the interpolation $I_h\bar{q}_k$ to be well-defined on the interval I_m. If the above condition is fulfilled for all time-intervals I_m, the following relation holds:

$$j_k'(\bar{q}_k)(\delta q - I_h\bar{q}_k) \geq 0 \quad \forall \delta q \in Q_{ad}. \tag{5.6}$$

Proof. The stability estimate from Proposition 4.1 and the fact that $\bar{q}_k \in Q_{\mathrm{ad}}$ imply that

$$k_m^{\frac{1}{2}} \|z_k(\bar{q}_k)(t_m)\|_{H^2(\Omega)} \leq C \quad \text{for } m = 1, 2, \ldots, M.$$

Due to a Sobolev embedding theorem and the choice of γ we have

$$\|z_k(\bar{q}_k)(t_m)\|_{C^{0,\gamma}(\bar{\Omega})} \leq C k_m^{-\frac{1}{2}} \quad \text{for } m = 1, 2, \ldots, M.$$

The projection $P_{Q_{\mathrm{ad}}} \colon C^{0,\gamma}(\bar{\Omega}) \to C^{0,\gamma}(\bar{\Omega})$ is continuous and therefore the optimality condition (3.9) implies

$$\|\bar{q}_k(t_m)\|_{C^{0,\gamma}(\bar{\Omega})} \leq \frac{C}{\alpha} k_m^{-\frac{1}{2}} \quad \text{for } m = 1, 2, \ldots, M.$$

Let x_i be a node in $\mathcal{T}_h$. Since the mesh $\mathcal{T}_h$ is quasi uniform, we have:

$$\max_{x \in \bar{\omega}(x_i)} \bar{q}_k(t_m, x) - \min_{x \in \bar{\omega}(x_i)} \bar{q}_k(t_m, x) \leq C \, \|\bar{q}_k(t_m)\|_{C^{0,\gamma}(\bar{\Omega})} h^\gamma \leq \frac{C}{\alpha} k_m^{-\frac{1}{2}} h^\gamma.$$

If this difference is below $q_b - q_a$ for all m, then $I_h\bar{q}_k$ is well-defined.

In order to show (5.6) we first consider a cell K with

$$\min_{x \in K} \bar{q}_k(t_m, x) = q_a.$$

Then we have $I_h\bar{q}_k(t_m) = q_a$ on K. Moreover, it holds $\bar{q}_k(t_m) < q_b$ on K for sufficiently small h by the same arguments as in the first part of the proof. This and the optimality condition (3.5) imply that

$$\alpha\bar{q}_k(t_m, x) + z_k(\bar{q}_k)(t_m, x) \geq 0 \quad \text{for } x \in K.$$

Therefore we obtain:

$$(\alpha\bar{q}_k(t_m, x) + z_k(\bar{q}_k)(t_m, x))(r - I_h\bar{q}_k(t_m, x)) \geq 0 \quad \text{for } q_a \leq r \leq q_b \text{ and } x \in K.$$

For the case

$$\max_{x \in K} \bar{q}_k(t_m, x) = q_b$$

we proceed similarly. On cells K with

$$q_a < q(t_m, x) < q_b \quad \text{for } x \in K,$$

we get by the optimality condition (3.5)

$$\alpha\bar{q}_k(t_m, x) + z_k(\bar{q}_k)(t_m, x) = 0 \quad \text{for } x \in K.$$

Integrating over all cells and time intervals leads to the desired result. ∎

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. Let moreover the conditions of Lemma 5.4 be fulfilled. Then the following estimate holds:*

$$\|\bar{q}_k - \bar{q}_\sigma\|_I \le \left(2 + \frac{C}{\alpha}\right) \|\bar{q}_k - I_h\bar{q}_k\|_I + \frac{1}{\alpha}\|z_k(\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I.$$

Proof. We split

$$\|\bar{q}_k - \bar{q}_\sigma\|_I \le \|\bar{q}_k - I_h\bar{q}_k\|_I + \|I_h\bar{q}_k - \bar{q}_\sigma\|_I,$$

and estimate the term $\|I_h\bar{q}_k - \bar{q}_\sigma\|_I$. Due to (3.15) we obtain for any $p \in Q$

$$\alpha\|I_h\bar{q}_k-\bar{q}_\sigma\|_I^2 \le j''_{kh}(p)(I_h\bar{q}_k-\bar{q}_\sigma, I_h\bar{q}_k-\bar{q}_\sigma) = j'_{kh}(I_h\bar{q}_k)(I_h\bar{q}_k-\bar{q}_\sigma)-j'_{kh}(\bar{q}_\sigma)(I_h\bar{q}_k-\bar{q}_\sigma).$$

The optimality condition (3.17) for $\bar{q}_\sigma$ and (5.6) imply the relation

$$-j'_{kh}(\bar{q}_\sigma)(I_h\bar{q}_k - \bar{q}_\sigma) \le 0 \le -j'_k(\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma).$$

Using the representations (3.6) of j'_k and (3.13) of j'_{kh} respectively, and Proposition 4.2 we obtain:

$$\begin{aligned}
\alpha\|I_h\bar{q}_k - \bar{q}_\sigma\|_I^2 &\le j'_{kh}(I_h\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma) - j'_k(\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma)\\
&= j'_{kh}(I_h\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma) - j'_{kh}(\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma)\\
&\quad + j'_{kh}(\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma) - j'_k(\bar{q}_k)(I_h\bar{q}_k - \bar{q}_\sigma)\\
&= (\alpha(I_h\bar{q}_k - \bar{q}_k) + (z_{kh}(I_h\bar{q}_k) - z_{kh}(\bar{q}_k)), I_h\bar{q}_k - \bar{q}_\sigma)_I\\
&\quad + (z_{kh}(\bar{q}_k) - z_k(\bar{q}_k), I_h\bar{q}_k - \bar{q}_\sigma)_I\\
&\le (C+\alpha)\|I_h\bar{q}_k - \bar{q}_k\|_I\|I_h\bar{q}_k - \bar{q}_\sigma\|_I\\
&\quad + \|z_k(\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I\|I_h\bar{q}_k - \bar{q}_\sigma\|_I.
\end{aligned}$$

This implies the desired estimate. ☐

In the next lemma we provide an estimate for the interpolation error $\|\bar{q}_k - I_h\bar{q}_k\|_I$.

LEMMA 5.6. *Let $\bar{q}_k \in Q_{ad}$ be the solution of the semidiscretized optimization problem* (3.4) *and $I_h\bar{q}_k$ be the interpolation constructed by* (5.5)*. Let moreover the conditions of Lemma 5.4 be fulfilled. Then, if Assumption 1 is fulfilled, the following estimate holds for $n < p \le \infty$ provided $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$:*

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

Proof. Since $I_h\bar{q}_k$ as well as $\bar{q}_k$ are piecewise constant in time we write

$$\|\bar{q}_k - I_h\bar{q}_k\|_I^2 = \sum_{m=1}^M \int_{I_m} \|\bar{q}_k(t) - I_h\bar{q}_k(t)\|^2\,dt = \sum_{m=1}^M k_m\|\bar{q}_k(t_m) - I_h\bar{q}_k(t_m)\|^2. \quad (5.7)$$

We start with

$$\begin{aligned}
&\|\bar{q}_k(t_m) - I_h\bar{q}_k(t_m)\|^2\\
&\qquad = \sum_{K\in\mathcal{T}_{h,m}^1} \|\bar{q}_k(t_m) - I_h\bar{q}_k(t_m)\|_{L^2(K)}^2 + \sum_{K\in\mathcal{T}_{h,m}^2} \|\bar{q}_k(t_m) - I_h\bar{q}_k(t_m)\|_{L^2(K)}^2.
\end{aligned}$$

For the first term we have:

$$\begin{aligned}\sum_{K\in\mathcal{T}^1_{h,m}} \|\bar q_k(t_m) - I_h\bar q_k(t_m)\|^2_{L^2(K)} &\le Ch^4 \sum_{K\in\mathcal{T}^1_{h,m}} \|\nabla^2 \bar q_k(t_m)\|^2_{L^2(K)}\\ &\le \frac{C}{\alpha^2} h^4 \|\nabla^2 z_k(\bar q_k)(t_m)\|^2,\end{aligned} \tag{5.8}$$

since $\bar q_k(t_m)$ equals either q_a, q_b, or $-\frac{1}{\alpha} z_k(\bar q_k)(t_m)$ on all cells $K \in \mathcal{T}^1_{h,m}$.

For cells $K \in \mathcal{T}^2_{h,m}$ we obtain either

$$\min_{x\in K} \bar q_k(t_m, x) = q_a \quad \text{and} \quad \max_{x\in K} \bar q_k(t_m, x) < q_b,$$

or

$$\max_{x\in K} \bar q_k(t_m, x) = q_b \quad \text{and} \quad \min_{x\in K} \bar q_k(t_m, x) > q_a.$$

As in the proof of Lemma 5.4 we have for the first case $I_h\bar q_k(t_m) = q_a$ on K. Since $W^{1,p}(K) \hookrightarrow C(K)$ for $p > n$, we may utilize standard interpolation estimates leading to

$$\begin{aligned}\|\bar q_k(t_m) - I_h\bar q_k(t_m)\|^2_{L^2(K)} = \|\bar q_k(t_m) - q_a\|^2_{L^2(K)} &\le |K|^{1-\frac{2}{p}} \|\bar q_k(t_m) - I_h\bar q_k(t_m)\|^2_{L^p(K)}\\ &\le Ch^2 |K|^{1-\frac{2}{p}} \|\nabla \bar q_k(t_m)\|^2_{L^p(K)}.\end{aligned}$$

The same estimate is obtained also for the second case. By summing up and using Assumption 1 we proceed:

$$\begin{aligned}\sum_{K\in\mathcal{T}^2_{h,m}} \|\bar q_k(t_m) - I_h\bar q_k(t_m)\|^2_{L^2(K)} &\le Ch^2 \sum_{K\in\mathcal{T}^2_{h,m}} |K|^{1-\frac{2}{p}} \|\nabla \bar q_k(t_m)\|^2_{L^p(K)}\\ &\le Ch^2 \left(\sum_{K\in\mathcal{T}^2_{h,m}} |K|\right)^{1-\frac{2}{p}} \|\nabla \bar q_k(t_m)\|^2_{L^p(\Omega)}\\ &\le \frac{C}{\alpha^2} h^{3-\frac{2}{p}} \|\nabla z_k(\bar q_k)(t_m)\|^2_{L^p(\Omega)}.\end{aligned} \tag{5.9}$$

Here we have used (3.9) and the continuity of the projection $P_{Q_{\mathrm{ad}}}\colon W^{1,p}(\Omega) \to W^{1,p}(\Omega)$. By inserting (5.8) and (5.9) in (5.7) we obtain the desired estimate. □

COROLLARY 5.7. *Under the conditions of Theorem 5.2 and Lemma 5.6 the following estimate holds:*

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

Proof. The result follows directly from Theorem 5.1, Theorem 5.5, Lemma 5.6, and Proposition 4.4. □

In the sequel we discuss the result from Corollary 5.7 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 $\bar q_k \in Q_{\mathrm{ad}}$, 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 $n < p \leq 6$ in three dimensions. This implies the order of convergence $\mathcal{O}\big(k + h^{\frac{3}{2}-\frac{1}{p}}\big)$ for all $n < p < \infty$ in 2d and $\mathcal{O}\big(k + h^{\frac{4}{3}}\big)$ in 3d, 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 $\mathcal{O}\big(k + h^{\frac{3}{2}}\big)$.

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 5.8. *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 5.9. *Let the conditions of Theorem 5.8 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 5.8 and the Propositions 4.3 and 4.4. □

5.4. Post-processing strategy. In this section, we extend the post-processing techniques initially proposed in [19] 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 post-processing 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 5.10. *Let $K \in \mathcal{T}_h$ be a given cell. Then we have*

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

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

- *and 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 [19] 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 5.11. *For a function $g_k \in X_k^0 \cap L^2(I, H^2)$ 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 5.10 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 5.12. *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

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

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 $\delta q = \bar{q}_\sigma$:

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

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

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

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

LEMMA 5.13. *Let $\bar q_k \in Q_{ad}$ be the solution of the semidiscrete optimization problem (3.4) and $\psi_{kh} \in X^{0,1}_{k,h}$. Let, moreover, Assumption 1 be fulfilled and $n < p \le \infty$. Then, it holds*

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

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 the continuity of the projection operator $P_{Q_{\text{ad}}} \colon H^1(\Omega) \to H^1(\Omega)$, we have for the first term

$$\begin{aligned} (\psi_{kh}, \bar q_k - \pi_d \bar q_k)_I = (\psi_{kh} - \pi_d \psi_{kh}, \bar q_k - \pi_d \bar q_k)_I &\le C h^2 \|\nabla \psi_{kh}\|_I \|\nabla \bar q_k\|_I \\ &\le \frac{C}{\alpha} h^2 \|\nabla \psi_{kh}\|_I \|\nabla z_k(\bar q_k)\|_I. \end{aligned} \tag{5.10}$$

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

$$\begin{aligned} &(\psi_{kh}(t_m), \pi_d \bar q_k(t_m) - R_d \bar q_k(t_m)) \\ &\quad = \sum_{K \in \mathcal{T}_h} \int_K \psi_{kh}(t_m, x)(\pi_d \bar q_k(t_m, x) - (R_d \bar q_k)(t_m, x))\, dx \\ &\quad = \sum_{K \in \mathcal{T}_h} \frac{1}{|K|} \int_K \psi_{kh}(t_m, x)\, dx \int_K (\pi_d \bar q_k(t_m, x) - (R_d \bar q_k)(t_m, x))\, dx \\ &\quad \le \|\psi_{kh}(t_m)\|_{L^\infty(\Omega)} \sum_{K \in \mathcal{T}_h} \left| \int_K (\bar q_k(t_m, x) - (R_d \bar q_k)(t_m, x))\, dx \right|. \end{aligned} \tag{5.11}$$

As in Section 5.2, we split the last sum using the separation $\mathcal{T}_h = \mathcal{T}^1_{h,m} \cup \mathcal{T}^2_{h,m}$ for $m = 1, 2, \dots, M$. For the sum over $\mathcal{T}^1_{h,m}$ we obtain by means of Lemma 5.10 and the fact that $\bar q_k(t_m)$ equals either q_a, q_b, or $-\frac{1}{\alpha} z_k(\bar q_k)(t_m)$:

$$\begin{aligned} \sum_{K \in \mathcal{T}^1_{h,m}} \left| \int_K (\bar q_k(t_m, x) - R_d \bar q_k(t_m, x))\, dx \right| &\le C h^2 \sum_{K \in \mathcal{T}^1_{h,m}} |K|^{\frac{1}{2}} \|\nabla^2 \bar q_k(t_m)\|_{L^2(K)} \\ &\le \frac{C}{\alpha} h^2 \|\nabla^2 z_k(\bar q_k)(t_m)\|. \end{aligned} \tag{5.12}$$

For the part of the sum over $\mathcal{T}_{h,m}^2$ the estimate of Lemma 5.10, Assumption 1, the optimality condition (3.9) and the continuity of the projection operator $P_{Q_{\mathrm{ad}}}$ on $W^{1,p}(\Omega)$ lead to

$$\begin{aligned}\sum_{K\in\mathcal{T}_{h,m}^2}\left|\int_K(\bar q_k(t_m,x)-R_d\bar q_k(t_m,x))\,dx\right| &\le \sum_{K\in\mathcal{T}_{h,m}^2}|K|^{1-\frac1p}\|\bar q_k(t_m)-R_d\bar q_k(t_m)\|_{L^p(K)}\\ &\le Ch\sum_{K\in\mathcal{T}_{h,m}^2}|K|^{1-\frac1p}\|\nabla\bar q_k(t_m)\|_{L^p(K)}\\ &\le \frac{C}{\alpha}h^{2-\frac1p}\|\nabla z_k(\bar q_k(t_m))\|_{L^p(\Omega)}.\end{aligned} \tag{5.13}$$

Inserting (5.12) and (5.13) into (5.11) and collecting the estimates (5.10) and (5.11) completes the proof. ∎

The following theorem provides a supercloseness result on the difference $R_d\bar q_k-\bar q_\sigma$:

THEOREM 5.14. *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. Let, moreover, Assumption 1 be fulfilled and $n<p\le\infty$. Then, it holds*

$$\begin{aligned}\|R_d\bar q_k-\bar q_\sigma\|_I \le \frac{C}{\alpha}h^2\Big\{\|\nabla^2u_k(\bar q_k)\|_I+\frac1\alpha\|\nabla z_k(\bar q_k)\|_I+\Big(1+\frac1\alpha\Big)\|\nabla^2z_k(\bar q_k)\|_I\Big\}\\ +\frac{C}{\alpha^2}h^{2-\frac1p}\|\nabla z_k(\bar q_k)\|_{L^2(I,L^p(\Omega))},\end{aligned}$$

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

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

$$\begin{aligned}\alpha\|R_d\bar q_k-\bar q_\sigma\|_I^2 &\le j_{kh}''(p)(R_d\bar q_k-\bar q_\sigma,R_d\bar q_k-\bar q_\sigma)\\ &= j_{kh}'(R_d\bar q_k)(R_d\bar q_k-\bar q_\sigma)-j_{kh}'(\bar q_\sigma)(R_d\bar q_k-\bar q_\sigma).\end{aligned}$$

By means of the inequality

$$-j_{kh}'(\bar q_\sigma)(R_d\bar q_k-\bar q_\sigma)\le 0\le -(\alpha R_d\bar q_k+R_dz_k(\bar q_k),R_d\bar q_k-\bar q_\sigma)_I,$$

which is implied by the optimality of $\bar q_\sigma$ and Lemma 5.12, and by means of the explicit representation of j_{kh}' from (3.13) we obtain

$$\begin{aligned}\alpha\|R_d\bar q_k-\bar q_\sigma\|_I^2 &\le (z_{kh}(R_d\bar q_k)-R_dz_k(\bar q_k),R_d\bar q_k-\bar q_\sigma)_I\\ &\le (z_{kh}(R_d\bar q_k)-z_k(\bar q_k),R_d\bar q_k-\bar q_\sigma)_I\\ &\quad+(z_k(\bar q_k)-R_dz_k(\bar q_k),R_d\bar q_k-\bar q_\sigma)_I.\end{aligned} \tag{5.14}$$

For the first term on the right-hand side of (5.14), we have by Cauchy's inequality

$$(z_{kh}(R_d\bar q_k)-z_k(\bar q_k),R_d\bar q_k-\bar q_\sigma)_I\le\|z_{kh}(R_d\bar q_k)-z_k(\bar q_k)\|_I\|R_d\bar q_k-\bar q_\sigma\|_I.$$

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

$$\|z_{kh}(R_d\bar q_k)-z_k(\bar q_k)\|_I\le\|z_{kh}(R_d\bar q_k)-z_{kh}(\bar q_k)\|_I+\|z_{kh}(\bar q_k)-z_k(\bar q_k)\|_I. \tag{5.15}$$

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

$$\|z_{kh}(R_d\bar{q}_k) - z_{kh}(\bar{q}_k)\|_I \le C\|u_{kh}(R_d\bar{q}_k) - u_{kh}(\bar{q}_k)\|_I. \tag{5.16}$$

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 5.13, we have

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

and the stability estimates from Proposition 4.2 and Lemma 4.5

$$\begin{aligned}\|\nabla(z_{kh}(q_k) - z_{kh}(R_dq_k))\|_I &\le C\|u_{kh}(R_dq_k) - u_{kh}(q_k)\|_I,\\ \|z_{kh}(q_k) - z_{kh}(R_dq_k)\|_{L^2(I,L^\infty(\Omega))} &\le C\|u_{kh}(R_dq_k) - u_{kh}(q_k)\|_I,\end{aligned}$$

yield the following intermediary result

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

We proceed by inserting this in (5.16) and in (5.15). This leads together with an estimate for the second term on the right-hand side of (5.15) from Proposition 4.4 to

$$\begin{aligned}\|z_{kh}(R_d\bar{q}_k) - z_k(\bar{q}_k)\|_I \le Ch^2\big\{&\|\nabla^2 u_k(\bar{q}_k)\|_I + \frac{1}{\alpha}\|\nabla z_k(\bar{q}_k)\|_I\\ &+ \Big(1+\frac{1}{\alpha}\Big)\|\nabla^2 z_k(\bar{q}_k)\|_I\big\} + \frac{C}{\alpha}h^{2-\frac{1}{p}}\|\nabla z_k(\bar{q}_k)\|_{L^2(I,L^p(\Omega))}.\end{aligned} \tag{5.17}$$

By applying Lemma 5.11 with $p_d = R_d\bar{q}_k - \bar{q}_\sigma$ to the second term on the right-hand side of (5.14), we get

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

The asserted result is obtained by insertion of the last two estimates into (5.14). ∎

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 post-processing step (3.18).

Corollary 5.15. *Let the conditions of Theorem 5.14 be fulfilled. Then, there holds:*

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

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

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

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

$$\alpha\|\bar{q} - \tilde{q}_\sigma\|_I \leq \|z(\bar{q}) - z_{kh}(\tilde{q}_\sigma)\|_I \leq \|z(\bar{q}) - z_k(\bar{q}_k)\|_I + \|z_k(\bar{q}_k) - z_{kh}(\tilde{q}_\sigma)\|_I. \tag{5.18}$$

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

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

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

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

Inserting the two last inequalities into (5.18) and applying the estimates from (5.17) and Theorem 5.14 yields the stated assertion. ◻

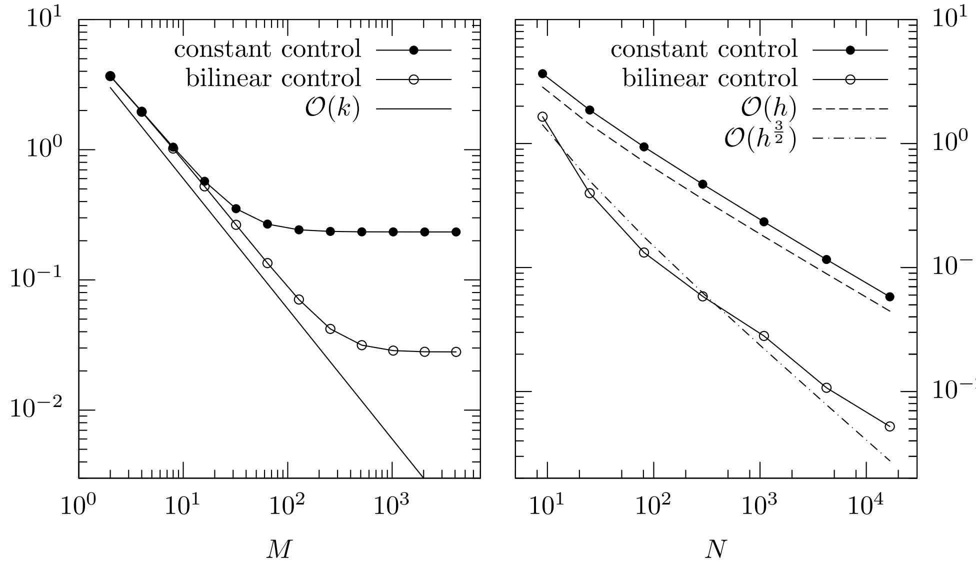
The choice of p in Corollary 5.15 follows the description in Section 5.2 requiring $z_k(\bar{q}_k) \in L^2(I, W^{1,p}(\Omega))$. Due to the fact that $\|z_k(\bar{q}_k)\|_{L^2(I,H^2(\Omega))}$ is bounded independently of k, the result in Corollary 5.15 holds for any $n < p < \infty$ in the two dimensional 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. Accordingly to the first part of this article [18], 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

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



(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* $\|\bar{q} - \bar{q}_\sigma\|_I$

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

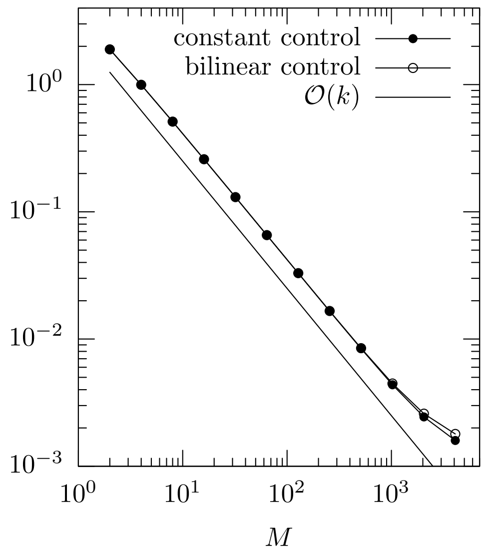
$$\begin{aligned}
\bar{q}(t, x_1, x_2) &:= P_{Q_{\mathrm{ad}}}\big(-\pi^4\{w_a(t, x_1, x_2) - w_a(T, x_1, x_2)\}\big),\\
\bar{u}(t, x_1, x_2) &:= \frac{-1}{2+a}\pi^2 w_a(t, x_1, x_2),\\
\bar{z}(t, x_1, x_2) &:= w_a(t, x_1, x_2) - w_a(T, x_1, x_2).
\end{aligned}$$

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. Secondly, we examine the behavior of the error under refinement of the spatial triangulation for $M = 2048$ time steps.

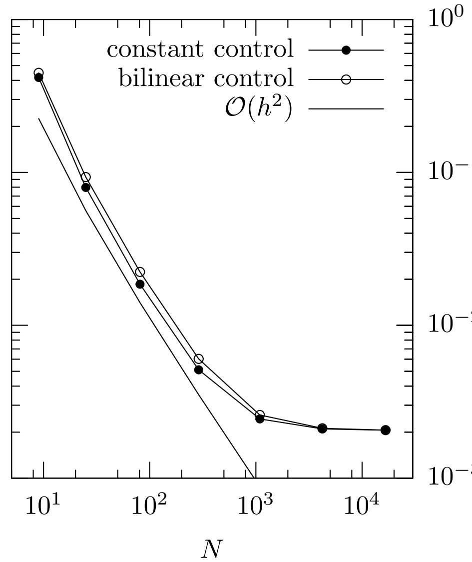
The state discretization is chosen as cG(1)dG(0), i.e., $r = 0$, $s = 1$. For the control discretization we use the same temporal and spatial meshes as for the state variable and present results for two choices of the discrete control space Q_d: cG(1)dG(0) and dG(0)dG(0). For the following computations,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

The optimal control problems are solved by the optimization library RoDoBo [20] using a primal-dual active set strategy (cf. [3, 12]) 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. For piecewise constant control (dG(0)dG(0) discretization), the discretization error is al-



(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* $\|\bar{u} - \bar{u}_\sigma\|_I$

ready 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 the 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) is observed. This illustrates the convergence results from the Sections 5.1 and 5.2 with respect to the *spatial* discretization.

The 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 proven in the previous section. Since the post-processing strategy presented in Section 5.4 relies essential on the convergence properties of the adjoint variable, Figure 6.3 confirms the proved order of convergence of the error $\|\bar{q} - \tilde{q}_\sigma\|_I$.

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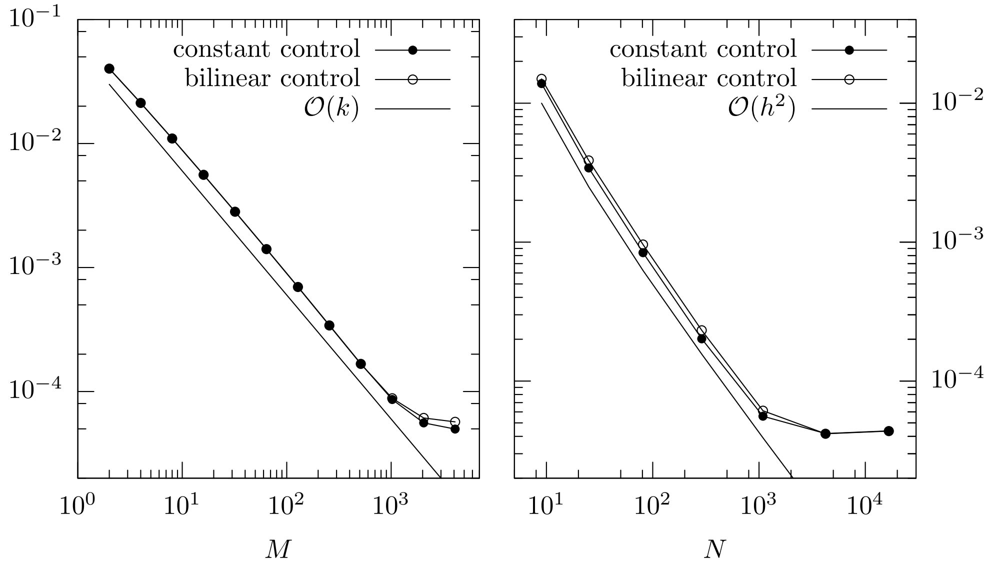

(a) Refinement of the time steps for $N = 1089$ spatial nodes

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

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

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