ERROR ESTIMATES FOR SPACE-TIME DISCRETIZATION OF PARABOLIC TIME-OPTIMAL CONTROL PROBLEMS WITH BANG-BANG CONTROLS*

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Abstract. In this paper a priori error estimates are derived for full discretization (in space and time) of time-optimal control problems. Various convergence results for the optimal time and the control variable are proved under different assumptions. Especially the case of bang-bang controls is investigated. Numerical examples are provided to illustrate the results.

Key words. Time-optimal control, Error estimates, Galerkin method, Bang-bang controls

AMS subject classifications. 49K20, 49M25, 65M15, 65M60

1. Introduction. In this article, we consider time-optimal control problems subject to parabolic partial differential equations. More precisely, we study the following model problem, where u denotes the state, q the control, and T the terminal time:

$$(P) \quad \text{Minimize } T \quad \text{subject to} \quad \begin{cases} T > 0, \\ \partial_t u - \Delta u = Bq, & \text{in } (0, T) \times \Omega, \\ u = 0, & \text{on } (0, T) \times \partial \Omega, \\ u(0) = u_0, & \text{in } \Omega, \\ G(u(T)) \le 0, \\ q_a \le q(t) \le q_b, & \text{in } \omega, t \in (0, T). \end{cases}$$

Here, we consider either distributed controls $q(t) \in L^2(\omega)$ for some appropriate subset $\omega \subset \Omega$ of the domain $\Omega \subset \mathbb{R}^d$, $d \in \{2, 3\}$, or parameter controls $q(t) \in \mathbb{R}^{N_c}$, $N_c \in \mathbb{N}$. Moreover, B is an appropriate control operator and $q_a, q_b \in \mathbb{R}$ are the control bounds; see Section 2 for the precise assumptions. The terminal constraint on the state is given by

(1.1)
$$G(u) \coloneqq \frac{1}{2} \|u - u_d\|_{L^2(\Omega)}^2 - \frac{\delta_0^2}{2},$$

where u_d denotes the desired state and $\delta_0 > 0$ is a given tolerance. Thus, the goal is to steer the heat-equation from an initial heat distribution u_0 as fast as possible into a ball of radius δ_0 around the desired state u_d . Without doubt, time-optimal control is a classical subject in control theory and we refer to, e.g., the monographs [20, 25, 16] for a general overview.

The aim of this article is to describe, for the first time, an appropriate fully spacetime discrete version of (P) and to prove *a priori* discretization error estimates. We note that the problem is posed on a variable time-horizon, which introduces a nonlinear dependency on the additional variable T. Furthermore, the optimal solutions to (P) are typically bang-bang (i.e. the set where the control does not equal the control

^{*}**Funding:** The first author gratefully acknowledge support from the International Research Training Group IGDK, funded by the German Science Foundation (DFG) and the Austrian Science Fund (FWF).

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bounds is a set of zero measure), since there are no control costs in the objective. This significantly complicates the numerical analysis of (P) compared to linear-quadratic problems with a fixed final time T considered in, e.g., [28, 29, 27] with control costs in the objective or [34] without control costs.

Even though time-optimal control problems have been extensively studied, there are a few publications concerning the discretization of this problem class in the context of parabolic equations. In [30, 22, 23, 37, 38, 18, 31, 21] the state equation is discretized in space only; see also the introduction of [5] for a detailed comparison. To the best of our knowledge, the only paper considering a full space-time discretization is [5] by the authors. However, in contrast to the aforementioned articles, an additional cost term

(1.2)
$$\frac{\alpha}{2} \|q\|_{L^2((0,T)\times\omega)}^2 \quad \text{with } \alpha > 0$$

is added to the objective functional in [5]. Unfortunately, the analysis given there does not apply in the case $\alpha = 0$. Moreover, the derived error estimates depend essentially on a *second order sufficient condition*, and the constants in the error estimates explode for $\alpha \to 0$. For this reason we cannot directly rely on those results.

To deal with the variable time horizon, the state and control variables are transformed to a reference interval. The state equation is discretized by means of the discontinuous Galerkin scheme in time and linear finite elements in space. We prove various convergence results; see also Table 1.1 for an overview. First, we show existence of solutions to the discrete problem and convergence of the optimal times $T_{kh} \rightarrow T$, where we only suppose that a linearized Slater condition on the continuous level holds. We emphasize that the latter condition is automatically satisfied in the setting with $u_d = 0$ and $0 \in Q_{ad}$ as considered in [22, 37, 31]; see [5, Theorem 3.10]. Second, if the optimal control is unique, then we show a convergence rate for the terminal time. For example, in the important special case of purely time-dependent controls, we obtain the optimal convergence rate $\mathcal{O}(k + h^2)$ for the optimal time (up to logarithmic factors). Here, k and h denote the temporal and spatial mesh size, respectively. In addition, we then assume that the following nodal set condition

(1.3)
$$|\{(t,x) \in I \times \omega : (B^*\bar{z})(t,x) = 0\}| = 0$$

holds. It requires the nodal set of the observation associated to the optimal adjoint state \bar{z} (see Lemma 3.2) to be of measure zero, where $|\cdot|$ denotes the measure associated with the product set $I \times \omega$. Based on (1.3) we prove further convergence results for the controls. Note that this condition, which is guaranteed for, e.g., the linear heat-equation with a distributed control (cf. also [31]), ensures uniqueness and the bang-bang property for the optimal control. Here, we generalize a technique based on a structural assumption of the adjoint state. Precisely, we show that the nodal set condition (1.3) implies the existence of a continuous function $\Psi: [0, \infty) \to [0, \infty)$ with $\Psi(0) = 0$ such that

(1.4)
$$|\{(t,x) \in I \times \omega \colon -\varepsilon \le (B^*\bar{z})(t,x) \le \varepsilon\}| \le \Psi(\varepsilon)$$

holds for all $\varepsilon > 0$. Based on (1.4), we derive an (abstract) growth condition. Furthermore, we prove that the nodal set condition (1.3) is a sufficient optimality condition (see Theorem 3.8), which seems to be a new result. Finally, assuming that the structural assumption (1.4) is valid with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$ for some constants $C, \kappa > 0$, we obtain the convergence rate $(k + h^2)^{\kappa}$ in L^1 for the control variable. In this way, we

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Assumptions	$ T_{kh} - T $	Control variable	Results
Linearized Slater condition + uniqueness of \bar{q} + nodal set condition (1.3) + (1.4) with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$	$ \begin{array}{l} \rightarrow 0 \\ \mathcal{O}\left(k+h^2\right) \\ \mathcal{O}\left(k+h^2\right) \\ \mathcal{O}\left(k+h^2\right) \end{array} $	$ \begin{array}{l} \stackrel{-}{\bar{q}_{kh}} \rightarrow \bar{q} \\ \bar{q}_{kh} \rightarrow \bar{q} \\ \left\ \bar{q}_{kh} - \bar{q} \right\ _{L^{1}} \lesssim \left(k + h^{2} \right)^{\kappa} \end{array} $	Lemma 4.3 Lemma 4.6 Theorem 4.8 Corollary 4.13, Theorem 4.15

TABLE 1.1

Summary of convergence results neglecting logarithmic terms. For simplicity we assume purely time-dependent control or distributed control with variational control discretization; see Corollary 4.19 for distributed control with piecewise and cellwise constant control.

are able to prove results which directly apply to the global solutions of the discrete problem, without requiring that they are chosen close to the (unique) continuous optimal solution.

Our results are improvements over existing contributions in different aspects. First, and most importantly, we deal with fully discrete problem formulations, which is crucial since it directly reflects how the problems are solved in practice. Neglecting this fact we compare our results to the literature in the following. In [22] an error estimate for the optimal times is proved that does not require uniqueness of the solution. However, in the particular case considered there the linearized Slater condition holds uniformly for the discrete problem, and this would also suffice for our argument; we also refer to [2, Section 5.6] for a generalization of [22] to fully discrete problems. For the case of a distributed control with the variational control discretization we can improve the result of [18] (see also [38] for a semilinear state equation) and obtain an optimal rate $\mathcal{O}(k+h^2)$. While the corresponding result from [37] with an explicit control discretization requires certain conditions (H1) and (H2), which so far could only be verified in very special situations, we assume a condition on the set of switchings which can be justified from practical observations; see Corollary 4.19. In [21] an error estimate of order $h^{2-\varepsilon}$ is obtained for a globally acting control and a semilinear state equation, whereas we can only prove $\mathcal{O}(k+h^{3/2})$. The reduced rate is due to control bounds in $L^{\infty}((0,T);L^2)$ instead of pointwise control constraints in time and space. Last, to the best of our knowledge, this article is the first one dealing with quantitative error estimates for the control variable in the context of time-optimal problems, using the structural assumption (1.4).

Finally, we comment on the validity of (1.4) with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$ for some $\kappa \in (0, 1]$. Although it is difficult to quantify the structural assumption a priori, we try to check it numerically, which serves as an indicator for the assumption for the continuous problem. In case of purely time-dependent controls, $\kappa = 1$ is valid in our examples and we observe the optimal order of convergence $\mathcal{O}(k+h^2)$ for the controls in L^1 . This is related to the fact that the N_c time-dependent functions constituting $B^*\bar{z}$ have only a finite number of simple roots; cf. Remark 3.6. In contrast, in case of a distributed control, the structural assumption only appears to be satisfied with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$ for some $\kappa < 1$ in our numerical tests, which restricts the rate of convergence. Here, we observe a better rate of convergence than expected for the value of κ that we estimated numerically. However, the optimal theoretical value of κ remains an open problem.

Concerning the numerical realization, we use the bilevel algorithm from [3] that is based on an equivalent reformulation of (P). In the outer loop we employ a Newton method to find the root of a certain value function. For the inner loop, we use an accelerated conditional gradient method. It is worth mentioning that this approach does not require a regularization term such as (1.2) in the objective.

This paper is organized as follows. In Section 2 we introduce the notation and main assumptions. Necessary and sufficient optimality conditions are discussed in Section 3. Section 4 is devoted to the discretization of the optimal control problem and the corresponding error estimates. In Section 5 we conclude with some numerical examples. The proposed algorithm is sketched in Appendix B.

2. Notation and main assumptions. We generally work with the same notation and assumptions as in [5] that will be summarized in the following for the convenience of the reader. For a Lipschitz domain $\Omega \subset \mathbb{R}^d$, let $H_0^1(\Omega)$ denote the usual Sobolev space with zero trace on the boundary. Its dual space is $H^{-1}(\Omega)$. We use $\langle \cdot, \cdot \rangle$ to denote the duality pairing between $H_0^1(\Omega)$ and $H^{-1}(\Omega)$. Usually we drop the spatial domain Ω from the notation of the function spaces, if ambiguity is not to be expected. For a Hilbert space Z, $(\cdot, \cdot)_Z$ stands for its inner product. Last, c is a generic constant that may have different values at different appearances.

Throughout this paper we impose the following assumptions.

ASSUMPTION 2.1. Let $\Omega \subset \mathbb{R}^d$, $d \in \{2,3\}$, be a polygonal or polyhedral and convex domain. Moreover, the initial value satisfies $u_0 \in H_0^1(\Omega)$.

Concerning the control operator B we consider one of the following situations:

- (i) Distributed control: Let $\omega \subseteq \Omega$ be the control domain that is polygonal or polyhedral as well. The control operator $B: L^2(\omega) \to L^2(\Omega)$ is the extension by zero and its adjoint $B^*: L^2(\Omega) \to L^2(\omega)$ is the restriction to ω operator.
- (ii) Purely time-dependent control: For $N_c \in \mathbb{N}$, let $\omega = \{1, 2, \dots, N_c\}$ be equipped with the counting measure. The control operator is defined by $Bq = \sum_{n=1}^{N_c} q_n e_n$, where $e_n \in L^2(\Omega)$ are given form functions. Then we have $L^2(\omega) \cong \mathbb{R}^{N_c}$ and $B^* \colon L^2(\Omega) \to \mathbb{R}^{N_c}$ with $(B^*\varphi)_n = (e_n, \varphi)_{L^2(\Omega)}$ for $n = 1, 2, \dots, N_c$.

The space of admissible controls is defined as

$$Q_{ad} \coloneqq \left\{ q \in L^2(\omega) \colon q_a \le q \le q_b \text{ a.e. in } \omega \right\} \subset L^{\infty}(\omega)$$

for $q_a, q_b \in \mathbb{R}$ with $q_a < q_b$. Moreover, for T > 0 we set $Q(0,T) := L^2((0,T) \times \omega)$ and

$$Q_{ad}(0,T) := \{q \in Q(0,T) : q(t) \in Q_{ad} \text{ a.e. } t \in (0,T)\} \subset L^{\infty}((0,T) \times \omega).$$

The set $(0,T) \times \omega$ is always equipped with the completion of the product measure. Furthermore, we use W(0,T) to abbreviate $H^1((0,T); H^{-1}) \cap L^2((0,T); H_0^1)$, endowed with the canonical norm and inner product. The symbol $i_T \colon W(0,T) \to H$ denotes the continuous trace mapping $i_T u = u(T)$. Last, the control operator B is extended to Q(0,T) by (Bq)(t) = Bq(t) for any $q \in Q(0,T)$.

ASSUMPTION 2.2. The terminal constraint G is defined by (1.1) for a fixed desired state $u_d \in H_0^1(\Omega)$ and $\delta_0 > 0$.

REMARK 2.1. The error analysis is also valid for more general terminal constraints. Concretely, we require that G is strictly convex, two times continuously Fréchet-differentiable, G'' is bounded on bounded sets in L^2 , and $G'(u)^* \in H_0^1$ for any $u \in H_0^1$. We focus on (1.1) to make the main ideas clearly visible to the reader.

In order to ensure existence of optimal solutions, we require

ASSUMPTION 2.3. There exist a finite time T > 0 and a feasible control $q \in Q_{ad}(0,T)$ such that the solution to the state equation of (P) satisfies $G(u(T)) \leq 0$. To exclude the trivial case, we additionally assume $G(u_0) > 0$.

PROPOSITION 2.2. If Assumption 2.3 holds, then there exists a globally optimal solution $(T, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, T)$ to (P). Moreover, the final time T and the observation $\bar{u}(T)$ are unique.

Proof. Existence follows by the direct method; cf. [5, Proposition 3.1]. Moreover, T is unique, because T is the objective functional. Last, uniqueness of $\bar{u}(T)$ follows from strict convexity of G and linearity of the control-to-observation mapping.

We also refer to [5, Remark 2.2] for a discussion of several situations where Assumption 2.3 is guaranteed to hold.

3. The time-optimal control problem. In this section we introduce the transformation approach, which forms the basis of the discretization concept, and collect results for the continuous problem (P) which are fundamental for the error analysis.

3.1. Change of variables. We transform the state equation to a fixed reference time interval in order to deal with the variable time horizon of (P). For $\nu \in \mathbb{R}_+$ we set $T_{\nu}(t) = \nu t$ and obtain the transformed state equation

$$\partial_t u - \nu \Delta u = \nu B q, \quad u(0) = u_0.$$

For each pair $(\nu, q) \in \mathbb{R}_+ \times Q(0, 1)$ there exists a unique solution to the transformed state equation; see, e.g., [12, Theorem 2, Chapter XVIII, §3]. Abbreviating I = (0, 1), let $S \colon \mathbb{R}_+ \times Q_{ad}(0, 1) \to W(I), (\nu, q) \mapsto u$, denote the corresponding control-to-state mapping. We define the reduced terminal constraint by

$$g(\nu, q) := G(i_1 S(\nu, q)),$$

where i_1 denotes the trace mapping. The transformed optimal control problem is

(P) Minimize
$$\nu$$
 subject to $g(\nu, q) \leq 0, (\nu, q) \in \mathbb{R}_+ \times Q_{ad}(0, 1).$

Note that both problems (P) and (\hat{P}) are equivalent; see, e.g., [4, Proposition 4.6]. Moreover, continuity of the trajectory $u: [0,1] \to L^2$ implies that the inequality constraint in (\hat{P}) can be replaced by an equality constraint, i.e. $g(\nu,q) = 0$. Otherwise a feasible control with a shorter time exists, which contradicts the optimality of the solution. Throughout the paper, we will need the following differentiability property, which is obtained by standard arguments; cf. also [5, Section 3.1].

LEMMA 3.1. Let $\nu \in \mathbb{R}_+$ and $q \in Q(0,1)$. The control-to-state mapping S is twice continuously Fréchet-differentiable. Moreover, $\delta u = S'(\nu,q)(\delta\nu,\delta q) \in W(0,1)$ is the unique solution to

$$\partial_t \delta u - \nu \Delta \delta u = \delta \nu (Bq + \Delta u) + \nu B \delta q, \quad \delta u(0) = 0,$$

for $(\delta\nu, \delta q) \in \mathbb{R} \times L^2(I \times \omega)$ and $\delta \tilde{u} = S''(\nu, q)(\delta\nu_1, \delta q_1; \delta\nu_2, \delta q_2) \in W(0, 1)$ is the unique solution to

$$\partial_t \delta \tilde{u} - \nu \Delta \delta \tilde{u} = \delta \nu_1 \left(B \delta q_2 + \Delta \delta u_2 \right) + \delta \nu_2 \left(B \delta q_1 + \Delta \delta u_1 \right), \quad \delta \tilde{u}(0) = 0,$$

for $(\delta \nu_i, \delta q_i) \in \mathbb{R} \times L^2(I \times \omega)$ and $\delta u_i = S'(\nu, q)(\delta \nu_i, \delta q_i), i = 1, 2.$

By means of Lemma 3.1, the reduced constraint mapping $g: \mathbb{R}_+ \times Q(0,1) \to \mathbb{R}$ is twice continuously Fréchet-differentiable. Moreover, the expressions

(3.1)
$$g'(\nu, q)(\delta\nu, \delta q) = (u(1) - u_d, \delta u(1))_{L^2}$$

(3.2)
$$g''(\nu,q)(\delta\nu_1,\delta q_1;\delta\nu_2,\delta q_2) = (\delta u_1(1),\delta u_2(1))_{L^2} + (u(1) - u_d,\delta \tilde{u}(1))_{L^2},$$

hold, where δu_1 , δu_2 , and $\delta \tilde{u}$ are defined as in Lemma 3.1. Last, for $\nu \in \mathbb{R}_+$, $q \in Q(0,1)$, $u = S(\nu, q)$, and $\mu \in \mathbb{R}$ we have the representation

(3.3)
$$\mu g'(\nu,q)^* = \begin{pmatrix} \int_0^1 \langle Bq + \Delta u, z \rangle \\ \nu B^* z \end{pmatrix}$$

where $z \in W(0, 1)$ is the unique solution to the adjoint state equation

$$-\partial_t z - \nu \Delta z = 0, \quad z(1) = \mu(u(1) - u_d).$$

3.2. First order necessary optimality conditions. We summarize first order optimality conditions from [5, Section 3.2] that also hold in the case without control costs in the objective functional. Let $(\bar{\nu}, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ be a solution to (\hat{P}) . We suppose that the following *linearized Slater* condition is satisfied.

ASSUMPTION 3.1. We assume that

(3.4)
$$\bar{\eta} \coloneqq -\partial_{\nu} g(\bar{\nu}, \bar{q}) > 0.$$

Note that due to Assumption 3.1 and $g(\bar{\nu}, \bar{q}) = 0$, the point $\check{\chi}^{\gamma} = (\bar{\nu} + \gamma, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ defined for $\gamma > 0$ satisfies

$$g(\bar{\chi}) + g'(\bar{\chi})(\bar{\chi}^{\gamma} - \bar{\chi}) = -\bar{\eta}\gamma < 0,$$

which is the typically used linearized Slater condition. Thus, we assume that this condition holds in a special form. As discussed in [5, Section 3.2] Assumption 3.1 is already equivalent to qualified first order optimality conditions. Hence, it is not restrictive to assume that the linearized Slater condition holds in the form (3.4).

To state optimality conditions, we introduce the Lagrange function as

$$\mathcal{L} \colon \mathbb{R}_+ \times Q(0,1) \times \mathbb{R} \to \mathbb{R}, \quad \mathcal{L}(\nu,q,\mu) \coloneqq \nu + \mu \, g(\nu,q).$$

Now, optimality conditions for (\hat{P}) in qualified form can be given as follows: For $\bar{\nu} > 0$ and $\bar{q} \in Q_{ad}(0,1)$ being a solution to (\hat{P}) there exists a $\bar{\mu} \ge 0$, such that

(3.5)
$$\partial_{(\nu,q)}\mathcal{L}(\bar{\nu},\bar{q},\bar{\mu})(\delta\nu,q-\bar{q}) \ge 0 \quad \text{for all } (\delta\nu,q) \in \mathbb{R} \times Q_{ad}(0,1).$$

Assumption 3.1 ensures the existence of a multiplier $\bar{\mu}$ that is always positive due to the special structure of the problem.

LEMMA 3.2. Let $(\bar{\nu}, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ be a solution of (\hat{P}) with associated state $\bar{u} = S(\bar{\nu}, \bar{q})$ and the linearized Slater condition (3.4) hold. Then there exists a multiplier $0 < \bar{\mu} \leq c/\bar{\eta}$ such that

(3.6)
$$\int_0^1 1 + \langle B\bar{q}(t) + \Delta\bar{u}(t), \bar{z}(t) \rangle \,\mathrm{d}t = 0,$$

(3.7)
$$\int_0^1 \langle B^* \bar{z}(t), q(t) - \bar{q}(t) \rangle \, \mathrm{d}t \ge 0 \quad \text{for all } q \in Q_{ad}(0,1),$$

(3.8)
$$G(\bar{u}(1)) = 0,$$

where the adjoint state $\bar{z} \in W(0,1)$ is determined by

(3.9)
$$-\partial_t \bar{z}(t) - \bar{\nu} \Delta \bar{z}(t) = 0, \quad t \in (0,1) \quad \bar{z}(1) = \bar{\mu}(\bar{u}(1) - u_d).$$

Proof. Note first that the linearized Slater condition allows for exact penalization of (\hat{P}) ; see [6, Theorem 2.87, Proposition 3.111]. The optimality conditions now follow as in the proof of [4, Theorem 4.12]. The condition (3.6) is equivalent to $\partial_{\nu} \mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu}) = 0$ and (3.7) arises from (3.5) for $\delta \nu = 0$. Last, we observe that $\bar{\mu} = 0$ implies $\bar{z} = 0$, which contradicts (3.6). Thus, $\bar{\mu} > 0$ must hold.

We emphasize that the adjoint state from Lemma 3.2 is unique up to multiplication by the positive scalar $\bar{\mu}$ due to uniqueness of the observation; see Proposition 2.2.

From the variational inequality (3.7) we infer that

(3.10)
$$(B^*\bar{z})(t,x) \begin{cases} \geq 0 & \text{for } \bar{q}(t,x) = q_a, \\ \leq 0 & \text{for } \bar{q}(t,x) = q_b, \\ = 0 & \text{for } q_a < \bar{q}(t,x) < q_b. \end{cases}$$

In this article we are interested in the case when \bar{q} is a bang-bang control, which is implied by the following condition:

ASSUMPTION 3.2. We assume that the nodal set condition

$$|\{(t,x) \in I \times \omega : (B^*\bar{z})(t,x) = 0\}| = 0$$

holds, where $|\cdot|$ denotes the measure associated with $I \times \omega$.

PROPOSITION 3.3. If Assumption 3.2 holds, then \bar{q} is bang-bang and unique.

Proof. From the optimality condition (3.10) and Assumption 3.2 we immediately infer that \bar{q} is a bang-bang control. To show uniqueness, let $q \in Q_{ad}(0,1)$ be a different optimal control. Set $q_{\lambda} = \lambda q + (1 - \lambda)\bar{q} \in Q_{ad}(0,1)$ for any $\lambda \in [0,1]$. Affine linearity of the control-to-state mapping for fixed ν and convexity of the terminal constraint imply that the pair $(\bar{\nu}, q_{\lambda})$ is also feasible for (\hat{P}) . In addition, a simple contradiction argument reveals that $(\bar{\nu}, q_{\lambda})$ is also optimal, i.e. $g(\bar{\nu}, q_{\lambda}) = 0$. Hence,

$$\bar{\nu} \int_0^1 \int_\omega B^* \bar{z}(q-\bar{q}) = \partial_q \mathcal{L}(\bar{\nu},\bar{q},\bar{\mu})(q-\bar{q}) = \lim_{\substack{\lambda \in (0,1]\\\lambda \to 0}} \frac{1}{\lambda} \left[\mathcal{L}(\bar{\nu},q_\lambda,\bar{\mu}) - \mathcal{L}(\bar{\nu},\bar{q},\bar{\mu}) \right] = 0.$$

With (3.10) and $q \in Q_{ad}(0,1)$, the integrand on the left-hand side is nonnegative. Thus, using $\bar{\nu} > 0$, it is zero almost everywhere. Finally, Assumption 3.2 implies $q = \bar{q}$, so \bar{q} is unique.

REMARK 3.4. We comment on situations in which Assumption 3.2 is guaranteed to hold.

- (i) In the case of a distributed control on an open subset $\omega \subset \Omega$, Assumption 3.2 is satisfied; see [16, Theorem 4.7.12]. Note that [19, Theorem 1.1] is only applied for interior subsets of the cylinder $I \times \Omega$. Employing interior regularity of the solution to the heat-equation with zero right-hand side, the general boundary regularity of this article is sufficient for the argument.
- (ii) Suppose purely time-dependent controls, i.e. $B: \mathbb{R}^{N_c} \to H^{-1}$, $Bq = \sum_{i=1}^{N_c} q_i e_i$ and set $B_i: \mathbb{R} \to H^{-1}$, $B_i q = q e_i$. If $(-\Delta, B_i)$ is approximately controllable for all i = 1, 2, ..., M, i.e. $q \mapsto \int_0^1 e^{(1-s)\Delta} B_i q(s) ds$ has dense range in $L^2(\Omega)$, then

Assumption 3.2 holds. This follows from analyticity of the semigroup generated by Δ and [32, Theorem 11.2.1, Definition 6.1.1]. In the context of time-optimal control of ODEs, approximate controllability of $(-\Delta, B_i)$ for all *i* is referred to as normality; see, e.g., [20, Section II.16] or [25, Section III.3].

We note that the assumption of normality implies that the Dirichlet Laplacian on the domain Ω has simple spectrum (all eigenvalues have geometric multiplicity one); see, e.g., [1, Theorem 1.3]. Unfortunately, this is not fulfilled for all domains – we refer to [1, Section 3.4] for a thorough discussion. While this limits the applicability of the above criterion to certain domains, we emphasize that it is only a sufficient condition.

3.3. Sufficient optimality conditions for bang-bang controls. Let $(\bar{\nu}, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ such that the necessary optimality conditions from Lemma 3.2 hold with $\bar{z} \in W(0, 1)$ the adjoint state $\bar{\mu} > 0$ the Lagrange multiplier.

PROPOSITION 3.5. Let Assumption 3.2 hold. Then there exists a concave, continuous, strictly monotonically increasing function $\Psi \colon [0,\infty) \to [0,\infty)$ with $\Psi(0) = 0$ and $\lim_{\varepsilon \to \infty} \Psi(\varepsilon) = \infty$ such that for all $\varepsilon > 0$ it holds

$$(3.11) |\{(t,x) \in I \times \omega \colon -\varepsilon \le (B^*\bar{z})(t,x) \le \varepsilon\}| \le \Psi(\varepsilon).$$

Proof. Define $\Phi(\varepsilon) := |\{(t, x) \in I \times \omega : -\varepsilon \leq (B^* \overline{z})(t, x) \leq \varepsilon\}|$, which is the lefthand side of (3.11). Then, $0 \leq \Phi(\varepsilon) \leq |I \times \omega| < \infty$. Moreover, one easily shows that Φ is continuous from the right, thus, in particular we have $\lim_{\varepsilon \searrow 0} \Phi(0) = 0$. Now, we define the concave hull of Φ by $\widetilde{\Phi} = -((-\Phi)^*)^*$, where $(\cdot)^*$ denotes the convex conjugate (also known as Fenchel-Legendre transform). Concretely,

$$\widetilde{\varPhi}(\varepsilon) = -\sup_{\gamma \in \mathbb{R}} \left[\varepsilon \gamma - \sup_{\varepsilon' \geq 0} (\varepsilon' \gamma + \varPhi(\varepsilon')) \right] = \inf_{\gamma \geq 0} \left[\varepsilon \gamma + \sup_{\varepsilon' \geq 0} (\varPhi(\varepsilon') - \varepsilon' \gamma) \right],$$

where, in the last line we have substituted γ by $-\gamma$. By the standard properties of the concave hull (see, e.g., [11, Corollary 4.22]), we have

(3.12)
$$\Phi(\varepsilon) \ge \Phi(\varepsilon) \quad \text{for all } \varepsilon \ge 0,$$

and $\widetilde{\Phi}$ is upper semi-continuous. Furthermore, we can verify that

$$\widetilde{\varPhi}(0) = \inf_{\gamma \ge 0} \sup_{\varepsilon' \ge 0} (\varPhi(\varepsilon') - \varepsilon' \gamma) = 0.$$

First, $\tilde{\Phi}(0) \geq 0$ follows from (3.12) and Assumption 3.2. Assume that $\tilde{\Phi}(0) > 0$. Then for each $\gamma > 0$ there is $\varepsilon = \varepsilon(\gamma) > 0$ such that $\tilde{\Phi}(0) \leq \Phi(\varepsilon) - \varepsilon\gamma + \tilde{\Phi}(0)/2$. Hence, $\tilde{\Phi}(0)/2 \leq \Phi(\varepsilon)$ and $\varepsilon < \Phi(\varepsilon)/\gamma$. Using the boundedness of Φ , we find $\varepsilon(\gamma) \to 0$ for $\gamma \to \infty$. However, $\lim_{\varepsilon \to 0} \Phi(\varepsilon) = 0$ which is a contradiction to $\tilde{\Phi}(0)/2 \leq \Phi(\varepsilon)$. Finally, $\tilde{\Phi}$ is continuous, since it is Lipschitz-continuous on $(0, \infty)$ (see, e.g., [11, Theorem 2.34]) and $\lim_{\varepsilon \to 0} \tilde{\Phi}(\varepsilon) = 0$ with upper semi-continuity. We conclude the proof by setting $\Psi(\varepsilon) = \tilde{\Phi}(\varepsilon) + \varepsilon$ to guarantee strict monotonicity and $\lim_{\varepsilon \to \infty} \Psi(\varepsilon) = \infty$.

REMARK 3.6. (i) In related contexts, the condition (3.11) is an assumption; see, e.g., [36, 13, 35, 10, 33, 34, 9] for the special case $\Psi(\varepsilon) = C\varepsilon^{\kappa}$ with constants C > 0 and $\kappa > 0$. However, we derived the existence of such a function Ψ , requiring only the nodal set condition from Assumption 3.2, which is guaranteed in many examples. (ii) In the context of a distributed control, where $B^*\bar{z} = \bar{z}|_{I \times \omega}$, a sufficient condition for a strong form of (3.11) is often given as follows (see, e.g., [13, Lemma 3.2]): Assume $\bar{z} \in C^1(\overline{I \times \omega})$ and that there exists a constant c > 0 such that

$$\left\|\nabla_{(t,x)}\bar{z}(t,x)\right\|_{\mathbb{R}^{d+1}} \ge c$$

for all $(t, x) \in I \times \omega$ such that $\overline{z}(t, x) = 0$, then (3.11) holds with $\Psi(\varepsilon) = C\varepsilon$.

(iii) Condition (3.11) is also compatible with purely time-dependent controls. In this case the structural condition concretely reads as

$$\sum_{n=1}^{N_c} |\{ t \in I \colon |(B^*\bar{z}(t))_n| \le \varepsilon \}| \le \Psi(\varepsilon).$$

In the context of optimal control problems with ODEs, the functions $t \mapsto \sigma_n(t) = (B^*\bar{z}(t))_n = (e_n, \bar{z}(t))_{L^2(\Omega)}$ are referred to as switching functions. Here, one typically assumes that each σ_n has only finitely many roots with non-vanishing first derivatives (see, e.g., [17, 26]), which again implies (3.11) with $\Psi(\varepsilon) = C\varepsilon$.

Clearly, any function Ψ with the properties as given in Proposition 3.5 possesses a convex, strictly monotonously increasing and continuous inverse $\Psi^{-1}: [0, \infty) \to [0, \infty)$ with $\Psi^{-1}(0) = 0$ and $\lim_{x\to\infty} \Psi^{-1}(x) = \infty$. The proof of sufficiency of the structural assumption for a pair $(\bar{\nu}, \bar{q})$ to be locally optimal relies now on the following result.

PROPOSITION 3.7. Let $(\bar{\nu}, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ satisfy the necessary optimality conditions from Lemma 3.2. Moreover, suppose that Assumption 3.2 holds. Then there is $c_0 > 0$ such that

(3.13)
$$\partial_q \mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu})(q - \bar{q}) \ge \frac{\bar{\nu}}{2} \Psi^{-1} \left(c_0 \|q - \bar{q}\|_{L^1(I \times \omega)} \right) \|q - \bar{q}\|_{L^1(I \times \omega)}$$

for all $q \in Q_{ad}(0,1)$, where Ψ is from Proposition 3.5.

Proof. The proof is along the lines of [10, Proposition 2.7] with slight modifications. For $q \in Q_{ad}(0, 1)$, we take $\varepsilon := \Psi^{-1}((2|q_b - q_a|)^{-1} ||q - \bar{q}||_{L^1(I \times \omega)})$. Now the estimate follows as in [10] with $c_0 = (2|q_b - q_a|)^{-1}$.

Assumption 3.2 allows to prove the following growth condition without two norm discrepancy. In particular, we infer that the nodal set condition is a sufficient optimality condition for the time-optimal control problem (P). It is worth mentioning that due to the particular objective functional we do not require additional assumptions such as conditions on the second derivative of the Lagrange function; cf. [8, Theorem 2.2] and [10, Theorem 2.8].

THEOREM 3.8. Let $(\bar{\nu}, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ satisfying first order necessary optimality conditions. Moreover, suppose that Assumption 3.2 holds. Then $(\bar{\nu}, \bar{q})$ is optimal for (\hat{P}) and there exists a constant $\delta > 0$ such that

(3.14)
$$\frac{\bar{\nu}}{6}\Psi^{-1}\left(c_{0}\|q-\bar{q}\|_{L^{1}(I\times\omega)}\right)\|q-\bar{q}\|_{L^{1}(I\times\omega)} \leq \nu-\bar{\nu}$$

for all admissible $(\nu, q) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$, i.e. $g(\nu, q) \leq 0$, with $|\nu - \bar{\nu}| \leq \delta$.

REMARK 3.9. In particular, the result from Theorem 3.8 implies that $\nu > \bar{\nu}$ for any admissible (ν, q) with $q \neq \bar{q}$, i.e., the optimal control \bar{q} is unique.

In order to prove the result, we first observe that the second derivative of the Lagrange function can be bounded below as follows.

PROPOSITION 3.10. Let $(\bar{\nu}, \bar{q}) \in \mathbb{R}_+ \times Q_{ad}(0, 1), \ \bar{\mu} > 0, \ and \ 0 < \nu_{\min} < \nu_{\max}$. There is c > 0 such that

$$\partial_{(\nu,q)}^2 \mathcal{L}(\nu_{\xi}, q_{\xi}, \bar{\mu}) [\nu - \bar{\nu}, q - \bar{q}]^2 \ge -c|\nu - \bar{\nu}|^2 - c|\nu - \bar{\nu}| \|q - \bar{q}\|_{L^2(I \times \omega)}$$

for all $\nu, \nu_{\xi} \in \mathbb{R}_+$, $q, q_{\xi} \in Q_{ad}(0,1)$ with $\nu_{\min} \leq \nu, \nu_{\xi} \leq \nu_{\max}$.

Proof. Set $\delta \nu = \nu - \bar{\nu}$ and $\delta q = q - \bar{q}$. Define $u_{\xi} = S(\nu_{\xi}, q_{\xi}), \, \delta u = S'(\nu_{\xi}, q_{\xi})(\delta \nu, \delta q)$, and $\delta \tilde{u} = S''(\nu_{\xi}, q_{\xi})[\delta \nu, \delta q]^2$. Moreover, let z_{ξ} be the corresponding adjoint state with terminal value $\bar{\mu}(u_{\xi}(1) - u_d)$. Then we observe

$$\begin{split} \bar{\mu}(u_{\xi}(1) - u_{d}, \delta \tilde{u}(1))_{L^{2}} &= (z_{\xi}(1), \delta \tilde{u}(1))_{L^{2}} - (z_{\xi}(0), \delta \tilde{u}(0))_{L^{2}} \\ &= \int_{0}^{1} \langle \partial_{t} \delta \tilde{u}, z_{\xi} \rangle + \int_{0}^{1} \langle \partial_{t} z_{\xi}, \delta \tilde{u} \rangle = \int_{0}^{1} \langle \partial_{t} \delta \tilde{u}, z_{\xi} \rangle - \int_{0}^{1} \langle \bar{\nu} \Delta \delta \tilde{u}, z_{\xi} \rangle \\ &= 2\delta \nu \int_{0}^{1} \langle B \delta q + \Delta \delta u, z_{\xi} \rangle \, \mathrm{d}t. \end{split}$$

Thus, using (3.2), we find

$$\partial_{(\nu,q)}^{2} \mathcal{L}(\nu_{\xi}, q_{\xi}, \bar{\mu}) [\delta\nu, \delta q]^{2} = \bar{\mu} \|\delta u(1)\|_{L^{2}}^{2} + 2\delta\nu \int_{0}^{1} \langle B\delta q + \Delta\delta u, z_{\xi} \rangle \,\mathrm{d}t$$
$$\geq -2|\delta\nu| \int_{0}^{1} |\langle B\delta q + \Delta\delta u, z_{\xi} \rangle| \,\mathrm{d}t.$$

The Cauchy-Schwarz inequality and the stability estimates for $u_{\xi}, \delta u$, and z_{ξ} with Lemma 3.1 further imply

$$\begin{aligned} \partial_{(\nu,q)}^{2} \mathcal{L}(\nu_{\xi}, q_{\xi}, \bar{\mu}) [\delta\nu, \delta q]^{2} &\geq -2|\delta\nu| \left(\|B\delta q\|_{L^{2}(I; H^{-1})} + \|\delta u\|_{L^{2}(I; H^{1}_{0})} \right) \|z_{\xi}\|_{L^{2}(I; H^{1}_{0})} \\ &\geq -c|\delta\nu| \left(\|B\delta q\|_{L^{2}(I; H^{-1})} + \frac{|\delta\nu|}{\nu_{\xi}} \left(\|Bq_{\xi}\|_{L^{2}(I; H^{-1})} + \|u_{\xi}\|_{L^{2}(I; H^{1}_{0})} \right) \right) \|z_{\xi}(1)\|_{L^{2}}. \end{aligned}$$

Since q_{ξ} is uniformly bounded due to boundedness of $Q_{ad}(0,1)$ and ν_{ξ} is uniformly bounded from below and from above, there exists a constant c > 0 such that

$$\partial_{(\nu,q)}^2 \mathcal{L}(\nu_{\xi}, q_{\xi}, \bar{\mu}) [\delta\nu, \delta q]^2 \ge -c |\delta\nu|^2 - c |\delta\nu| \|\delta q\|_{L^2(I \times \omega)}$$

proving the assertion.

Last, we require a technical result, which follows from the Fenchel-Young inequality.

PROPOSITION 3.11. Let $\varepsilon > 0$, $c_0 > 0$, and let Ψ satisfy the assumptions of Proposition 3.5. Then there exists a (convex) function $F: [0, \infty) \to [0, \infty)$ such that

$$xy \le \varepsilon \Psi^{-1}(c_0 x^2) x^2 + F(y) \quad \text{for all } x, y \in [0,\infty),$$

and F(0) = 0 and $\lim_{y\to 0} F(y)/y = 0$.

Proof. We abbreviate $H(x) = \varepsilon \Psi^{-1}(c_0 x^2) x^2$. Note first that Ψ^{-1} is convex as the inverse of a concave function. Thus, it is Lipschitz continuous on the interior of its domain \mathbb{R}_+ ; see, e.g., [11, Theorem 2.34]. Therefore, we can apply Rademacher's theorem and the chain rule to compute the derivative

$$H'(x) = 2\varepsilon \left(c_0 (\Psi^{-1})' (c_0 x^2) x^3 + \Psi^{-1} (c_0 x^2) x \right),$$

which is defined almost everywhere. Using again that Ψ^{-1} is convex, we verify that H' is monotonically increasing. Hence, H is convex, locally Lipschitz continuous, and strictly monotonically increasing. Now, we define $F = H^*$, where $H^*(y) = \sup_{x\geq 0} [yx - H(x)]$ is the convex conjugate of H. Clearly, $F(y) \geq F(0) = H(0) = 0$ for all $y \geq 0$. Thus, the desired inequality is given by the Fenchel-Young inequality $xy \leq H(x) + H^*(y)$.

It remains to verify that the directional derivative of F at zero, i.e. $F'(0,+1) = \lim_{y\to 0} (F(y) - F(0))/(y - 0) = \lim_{y\to 0} F(y)/y$, is equal to zero. We consider the subdifferential $\partial F(0)$, which reads in this case as

$$\partial F(0) = \{ v \in \mathbb{R} \colon F(x) / x \ge v \text{ for all } x > 0 \}$$

Assume that F'(0,+1) > 0. Then $(-\infty, F'(0,+1)] \subset \partial F(0)$. Therefore, we deduce that $0 \in \partial H(x)$ for all $x \leq F'(0,+1)$ by the subdifferential inversion formula; see, e.g., [11, Exercise 4.27]. This implies that these points are global minima of H and thus H(x) = 0 for $x \leq F'(0,+1)$, which contradicts the strict monotonicity of H.

Finally, we are give the proof of the main result of this section.

Proof of Theorem 3.8.. Let $(\nu, q) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ be admissible. Set $\delta \nu = \nu - \bar{\nu}$ and $\delta q = q - \bar{q}$. Using feasibility of (ν, q) , the facts that $\bar{\mu} > 0$ and $g(\bar{\nu}, \bar{q}) = 0$ from the necessary optimality conditions for $(\bar{\nu}, \bar{q})$, as well as Taylor expansion we find

$$\begin{split} \nu - \bar{\nu} &\geq \nu + \bar{\mu}g(\nu, q) - (\bar{\nu} + \bar{\mu}g(\bar{\nu}, \bar{q})) = \mathcal{L}(\nu, q, \bar{\mu}) - \mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu}) \\ &= \partial_{(\nu, q)}\mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu})(\delta\nu, \delta q) + \frac{1}{2}\partial_{(\nu, q)}^2\mathcal{L}(\nu_{\xi}, q_{\xi}, \bar{\mu})[\delta\nu, \delta q]^2, \end{split}$$

with appropriate $\nu_{\xi} = \bar{\nu} + \xi_{\nu}(\nu - \bar{\nu})$ and $q_{\xi} = \bar{q} + \xi_q(q - \bar{q})$ for $0 \leq \xi_{\nu}, \xi_q \leq 1$. Thus, according to Proposition 3.10 there is $c_1 > 0$ such that

$$\nu - \bar{\nu} \ge \partial_{(\nu,q)} \mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu}) (\delta \nu, \delta q) - c_1 |\delta \nu|^2 - c_1 |\delta \nu| \|\delta q\|_{L^2(I \times \omega)}.$$

Since $\partial_{\nu} \mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu}) = 0$ and using Proposition 3.7, this further implies

$$\nu - \bar{\nu} \ge \frac{\bar{\nu}}{2} \Psi^{-1} \left(c_0 \|\delta q\|_{L^1(I \times \omega)} \right) \|\delta q\|_{L^1(I \times \omega)} - c_1 |\delta \nu|^2 - c_1 |\delta \nu| \|\delta q\|_{L^2(I \times \omega)}.$$

Clearly, we have

$$\|\delta q\|_{L^{2}(I\times\omega)} \leq \|\delta q\|_{L^{\infty}(I\times\omega)}^{1/2} \|\delta q\|_{L^{1}(I\times\omega)}^{1/2} \leq |q_{b} - q_{a}|^{1/2} \|\delta q\|_{L^{1}(I\times\omega)}^{1/2}$$

Employing Proposition 3.11 for some $\varepsilon > 0$ to determined later, we obtain

$$\|\delta\nu\| \|\delta q\|_{L^1(I\times\omega)}^{1/2} \le \varepsilon \Psi^{-1} \left(c_0 \|\delta q\|_{L^1(I\times\omega)} \right) \|\delta q\|_{L^1(I\times\omega)} + F(|\delta\nu|).$$

Taking $\varepsilon = \left(4c_1|q_b - q_a|^{1/2}\right)^{-1} \bar{\nu}$, we obtain

$$\delta\nu + F(|\delta\nu|) + c_1 |\delta\nu|^2 \ge \frac{\bar{\nu}}{4} \Psi^{-1} \left(c_0 \|q - \bar{q}\|_{L^1(I \times \omega)} \right) \|q - \bar{q}\|_{L^1(I \times \omega)}.$$

Finally, using that $\lim_{y\to 0} F(y)/y = 0$, we deduce

$$F(|\delta\nu|) + c_1 |\delta\nu|^2 \le \frac{1}{2} |\delta\nu|, \quad |\delta\nu| \le \delta,$$

for $\delta > 0$ sufficiently small, concluding the proof.

REMARK 3.12. For the special case $\Psi(\varepsilon) = C\varepsilon^{\kappa}$, in Proposition 3.7 we obtain

$$\partial_q \mathcal{L}(\bar{\nu}, \bar{q}, \bar{\mu})(q - \bar{q}) \ge c \|q - \bar{q}\|_{L^1(I \times \omega)}^{1 + 1/\kappa}$$

Moreover, the growth condition from Theorem 3.8 reads as follows: There are $\delta > 0$ and c > 0 such that

$$c \|q - \bar{q}\|_{L^1(I \times \omega)}^{1+1/\kappa} \le \nu - \bar{\nu}$$

for all admissible $(\nu, q) \in \mathbb{R}_+ \times Q_{ad}(0, 1)$ with $|\nu - \overline{\nu}| \leq \delta$.

4. A priori discretization error estimates. The aim of this section is the derivation of discretization error estimates for bang-bang controls based on the different conditions of the preceding section. We consider the same assumptions concerning the temporal and spatial discretization of the partial differential equation as in [5], which will be summarized in the following for the convenience of the reader. Let

$$[0,1] = \{0\} \cup I_1 \cup I_2 \cup \ldots \cup I_M$$

be a partitioning of the reference time interval [0,1] with disjoint subintervals $I_m = (t_{m-1}, t_m]$ of size k_m defined by the time points

$$0 = t_0 < t_1 < \ldots < t_{M-1} < t_M = 1$$

Moreover, let k denote the time discretization parameter defined as the piecewise constant function $k|_{I_m} = k_m$ for all m = 1, 2, ..., M. We also set $k = \max k_m$ the maximal time step size. The temporal mesh is assumed to be regular in the sense of [27, Section 3.1].

Concerning the spatial discretization, let $\mathcal{T}_h = \{K\}$ be a mesh consisting of triangular or tetrahedral cells K that form a non-overlapping cover of the domain Ω . The corresponding spatial discretization parameter h is the cellwise constant function $h|_K = h_K$, where h_K is the diameter of the cell K. In addition, we set $h = \max h_K$. Let $V_h \subset H_0^1$ denote the subspace of continuous and cellwise linear functions. We assume that the L^2 -projection onto V_h , denoted by $\Pi_h \colon L^2 \to V_h$, is stable in H^1 . This is satisfied if the mesh is globally quasi-uniform, but weaker conditions are known; see [7]. We construct the space-time finite element space in a standard way by setting

$$X_{k,h} = \left\{ v_{kh} \in L^2(I; V_h) \colon v_{kh} |_{I_m} \in \mathcal{P}_0(I_m; V_h), \ m = 1, 2, \dots, M \right\},\$$

where $\mathcal{P}_0(I_m; V_h)$ is the space of constant functions on the time interval I_m with values in V_h . Moreover, for $\varphi_k \in X_{k,h}$ we set $\varphi_{k,m} \coloneqq \varphi_k(t_m)$ with $m = 1, 2, \ldots, M$, as well as $[\varphi_k]_m \coloneqq \varphi_{k,m+1} - \varphi_{k,m}$ for $m = 1, 2, \ldots, M - 1$.

In order to introduce the discrete version to the state equation, let the trilinear form B: $\mathbb{R} \times X_{k,h} \times X_{k,h} \to \mathbb{R}$ be defined as

$$B(\nu, u_{kh}, \varphi_{kh}) \coloneqq \sum_{m=1}^{M} \langle \partial_t u_{kh}, \varphi_{kh} \rangle_{L^2(I_m; L^2)}$$
$$+ \nu (\nabla u_{kh}, \nabla \varphi_{kh})_{L^2(I; L^2)} + \sum_{m=2}^{M} ([u_{kh}]_{m-1}, \varphi_{kh,m}) + (u_{kh,1}, \varphi_{kh,1}).$$

Given $\nu \in \mathbb{R}_+$ and $q \in Q(0,1)$ the discrete state equation reads as follows: Find a state $u_{kh} \in X_{k,h}$ satisfying

(4.1)
$$B(\nu, u_{kh}, \varphi_{kh}) = \nu(Bq, \varphi_{kh})_{L^2(I;L^2)} + (u_0, \varphi_{kh,1})_{L^2} \text{ for all } \varphi_{kh} \in X_{k,h}$$

We also introduce the discrete Laplace operator $-\Delta_h: V_h \to V_h$ by

$$-(\Delta_h u_h, \varphi_h)_{L^2} = (\nabla u_h, \nabla \varphi_h)_{L^2}, \quad \varphi_h \in V_h$$

Next, we introduce a discrete control variable. To consider different discretization schemes in one consistent notation, we introduce the operator I_{σ} onto the possibly discrete control space $Q_{\sigma}(0,1) \subset L^2(I \times \omega)$, where σ is abstract parameter for the control discretization. To simplify the discussion, we assume that in the case of a distributed control a subset denoted \mathcal{T}_h^{ω} of the mesh \mathcal{T}_h is a non-overlapping cover of ω . Furthermore, we suppose that the optimal control \bar{q} satisfies

(4.2)
$$\|B(\bar{q} - I_{\sigma}\bar{q})\|_{L^{2}(I:H^{-1})} \leq \sigma(k,h)$$

where $\sigma(k,h) \to 0$ as $k,h \to 0$ and $I_{\sigma}Q_{ad}(0,1) \subset Q_{ad}(0,1)$. We also simply write $I_{\sigma}(\nu,q) = (\nu, I_{\sigma}q)$ using the same symbol and define $Q_{ad,\sigma}(0,1) = Q_{\sigma}(0,1) \cap Q_{ad}(0,1)$. Concrete discretization schemes for the control will be discussed at the end of this section.

We define the discretized optimal control problem corresponding to (P) by

$$(\hat{P}_{kh}) \qquad \qquad \text{Minimize } \nu_{kh} \quad \text{subject to} \quad \nu_{kh} \in \mathbb{R}_+, \ q_{kh} \in Q_{ad,\sigma}(0,1), \\ q_{kh}(\nu_{kh},q_{kh}) \leq 0, \end{cases}$$

where $g_{kh}(\nu_{kh}, q_{kh}) = G(i_1 S_{kh}(\nu_{kh}, q_{kh}))$ and S_{kh} denotes the control-to-state mapping for the discrete state equation (4.1). In the following, $\{(k, h)\}$ is always a sequence of positive mesh sizes converging to zero.

4.1. Error estimates for the terminal times. Similar as in [5] we construct two auxiliary sequences: First, we construct $\{(\nu_{\gamma}, q_{\gamma})\}_{\gamma>0}$ converging to $(\bar{\nu}, \bar{q})$ as $\gamma \to 0$ that is feasible for (\hat{P}_{kh}) . In particular, this ensures existence of a solution to the discrete problem. Moreover, we obtain a first convergence result without rates. Thereafter, we construct another sequence $\{(\nu_{\tau}, q_{\tau})\}_{\tau>0}$ converging to $(\bar{\nu}_{kh}, \bar{q}_{kh})$ as $\tau \to 0$ that is feasible for (\hat{P}) . Since the solution operator to the state equation is continuous for right-hand sides from $L^2(I; H^{-1})$ into $W(0, 1) \hookrightarrow C([0, 1]; L^2)$, we may use (4.2) for all estimates concerning the state or the linearized state. Note that all sequences constructed in [5] are independent of the cost parameter α .

For the error estimates, we require the following stability and discretization error estimates that are essentially based on [5, Propositions 4.4 and 4.6].

PROPOSITION 4.1. Let $0 < \nu_{\min} < \nu_{\max}$ be fixed. Then for all $\nu_{\min} \leq \nu \leq \nu_{\max}$ and $q \in Q_{ad}(0,1)$ we have

$$(4.3) \qquad \qquad |\partial_{\nu\nu}g_{kh}(\nu,q)| \le c_{\mu}$$

where c > 0 is a constant independent of ν , q, k, and h. Moreover,

(4.4)
$$|g(\nu,q) - g_{kh}(\nu,q)| \le c |\log k| (k+h^2) \left(\|Bq\|_{L^{\infty}(I;L^2)} + \|u_0\|_{L^2} \right),$$

(4.5)
$$|\partial_{\nu}g(\nu,q) - \partial_{\nu}g_{kh}(\nu,q)| \le c |\log k| (k+h^2) \left(\|Bq\|_{L^{\infty}(I;L^2)} + \|u_0\|_{H^1} \right),$$

where c > 0 is a constant independent of ν , q, k, and h.

PROPOSITION 4.2. Let $(\bar{\nu}, \bar{q})$ be a globally optimal control of problem (\bar{P}) . There exists a sequence $\{(\nu_{\gamma}, q_{\gamma})\}_{\gamma>0}$ of controls with $\gamma = \gamma(k, h)$ that are feasible for (\hat{P}_{kh}) for k and h sufficiently small. Moreover, we have the estimate

$$|\nu_{\gamma} - \bar{\nu}| \le c \left(\sigma(k, h) + |\log k| (k + h^2) \right).$$

Proof. The sequence can be constructed as in [5, Proposition 4.7]. We give the proof for convenience and abbreviate $\bar{\chi} = (\bar{\nu}, \bar{q})$. For $\gamma > 0$ to be determined in the course of the proof we set

$$\chi_{\gamma} \coloneqq \mathbf{I}_{\sigma} \breve{\chi}^{\gamma} = (\bar{\nu} + \gamma, \mathbf{I}_{\sigma} \bar{q}).$$

Using Taylor expansion of g_{kh} at $I_{\sigma}\bar{\chi}$ we find for some χ_{ζ} that

(4.6)
$$g_{kh}(\chi_{\gamma}) = g_{kh}(\mathbf{I}_{\sigma}\bar{\chi}) + \gamma g'_{kh}(\mathbf{I}_{\sigma}\bar{\chi})(1,0) + \frac{\gamma^2}{2} g''_{kh}(\chi_{\zeta})[1,0]^2.$$

Using the triangle inequality we estimate the first term of (4.6) by

(4.7)

$$g_{kh}(\mathbf{I}_{\sigma}\bar{\chi}) \leq g(\bar{\chi}) + |g_{kh}(\mathbf{I}_{\sigma}\bar{\chi}) - g(\mathbf{I}_{\sigma}\bar{\chi})| + |g(\mathbf{I}_{\sigma}\bar{\chi}) - g(\bar{\chi})| \\ \leq c |\log k|(k+h^2) + c||B(\mathbf{I}_{\sigma}\bar{q}-\bar{q})||_{L^2(I;H^{-1})} \\ \leq c_1(|\log k|(k+h^2) + \sigma(k,h)) \eqqcolon \delta_1(k,h)$$

with (4.4) and Lipschitz continuity of g. For the second term of (4.6), we estimate

(4.8)
$$g'_{kh}(\mathbf{I}_{\sigma}\bar{\chi})(1,0) \le g'(\bar{\chi})(1,0) + c_2\left(|\log k|(k+h^2) + \sigma(k,h)\right) \le -\bar{\eta} + \delta_2(k,h)$$

using Assumption 3.1, and $g'(\bar{\chi})(1,0) = \partial_{\nu}g(\bar{\chi})$. Finally, for the third term, we obtain $g''_{kh}(\chi_{\zeta})[\gamma,0]^2 \leq c_3\gamma^2$ due to (4.3). Collecting the estimates, we have

$$g_{kh}(\chi_{\gamma}) \leq \delta_1(k,h) - \gamma \left(\bar{\eta} - \delta_2(k,h) - c_3\gamma\right).$$

Note that the first component of χ_{γ} is bounded below by $\bar{\nu}$ and bounded above by $\bar{\nu} + 1$, so that all constants of the error and stability estimates used above can be chosen to be independent of χ_{γ} . Taking

$$\gamma = \frac{3\delta_1(k,h)}{\bar{\eta}} \le \frac{\bar{\eta}}{3c_3}$$
 and $\delta_2(k,h) \le \frac{\bar{\eta}}{3}$

for k, h sufficiently small, we obtain $g_{kh}(\chi_{\gamma}) \leq 0$. From the definition of γ we further deduce $\gamma = \gamma(k, h) = \mathcal{O}(\sigma(k, h) + |\log k|(k + h^2))$.

In particular, Proposition 4.2 implies existence of feasible points for the discrete problem (\hat{P}_{kh}) , which in turn guarantees existence of an optimal solution to the discrete problem. Even better, we obtain a first convergence result.

LEMMA 4.3. Let $(\bar{\nu}, \bar{q})$ be an optimal solution of problem (\hat{P}) such that Assumption 3.1 holds. For k and h sufficiently small, the discrete problem (\hat{P}_{kh}) has an optimal solution $(\bar{\nu}_{kh}, \bar{q}_{kh}) \in \mathbb{R}_+ \times Q_{ad,\sigma}(0,1)$. Moreover, $\bar{\nu}_{kh} \to \bar{\nu}$ and every weak limit of $(\bar{q}_{kh})_{k,h>0}$ is optimal for (\hat{P}) .

Proof. Existence of solutions follows by standard arguments, since the set of admissible controls is nonempty according to Proposition 4.2. Moreover, using optimality of $(\bar{\nu}_{kh}, \bar{q}_{kh})$, feasibility of $(\nu_{\gamma}, q_{\gamma})$, and $0 \leq \gamma \leq 1$, we observe

$$0 \le \bar{\nu}_{kh} \le \nu_{\gamma} = \bar{\nu} + \gamma \le \bar{\nu} + 1.$$

Hence, $(\bar{\nu}_{kh}, \bar{q}_{kh})$ is uniformly bounded. Thus, there exists a subsequence denoted in the same way such that $\bar{\nu}_{kh} \to \nu^*$ and $q_{kh} \rightharpoonup q^*$ in $L^s(I \times \omega)$ with $q^* \in Q_{ad}(0, 1)$ and

some s > 2. Feasibility of $(\bar{\nu}_{kh}, \bar{q}_{kh})$ for (\hat{P}_{kh}) further yields

$$g(\nu^*, q^*) \le g_{kh}(\bar{\nu}_{kh}, \bar{q}_{kh}) + |g(\bar{\nu}_{kh}, \bar{q}_{kh}) - g_{kh}(\bar{\nu}_{kh}, \bar{q}_{kh})| + |g(\nu^*, q^*) - g(\bar{\nu}_{kh}, \bar{q}_{kh})| \\ \le c \|i_1 S(\bar{\nu}_{kh}, \bar{q}_{kh}) - i_1 S_{kh}(\bar{\nu}_{kh}, \bar{q}_{kh})\|_{L^2} + c \|i_1 S(\nu^*, q^*) - i_1 S(\bar{\nu}_{kh}, \bar{q}_{kh})\|_{L^2},$$

where we have used Lipschitz continuity of G on bounded sets in L^2 . Going to the limit $k, h \to 0$, employing the convergence result Proposition A.5 as well as complete continuity Proposition A.1, we deduce that $g(\nu^*, q^*) \leq 0$. In particular, $\bar{\nu} \leq \nu^*$.

Optimality of $(\bar{\nu}_{kh}, \bar{q}_{kh})$ and feasibility of $(\nu_{\gamma}, q_{\gamma})$ from Proposition 4.5 for (\hat{P}_{kh}) , leads to

$$\nu^* = \lim_{k,h \to 0} \bar{\nu}_{kh} \le \lim_{k,h \to 0} \nu_{\gamma} = \lim_{k,h \to 0} \bar{\nu} + c \left(\sigma(k,h) + |\log k| (k+h^2) \right) = \bar{\nu}.$$

Hence, $\bar{\nu} = \nu^*$ and $(\bar{\nu}, q^*)$ is also optimal. Moreover, as the limit $\bar{\nu}$ is independent of the concretely chosen subsequence, the whole sequence converges.

In addition, Lemma 4.3 implies that the sequence $\bar{\nu}_{kh}$ is uniformly bounded away from zero. Hence, the constants in the following error estimates can be chosen to be independent of $\bar{\nu}_{kh}$; cf. Proposition 4.1 and Lemma A.4.

As the next step towards error estimates, we verify that the linearized Slater condition holds at $(\bar{\nu}_{kh}, \bar{q}_{kh})$ for the discrete problem. From now on we assume uniqueness of the optimal solution; recall Assumption 3.2 and Proposition 3.3 for a sufficient condition.

PROPOSITION 4.4. Let $(\bar{\nu}, \bar{q})$ be the unique optimal solution of (\hat{P}) such that Assumption 3.1 holds. Moreover, let $(\bar{\nu}_{kh}, \bar{q}_{kh}) \in \mathbb{R}_+ \times Q_{ad,\sigma}(0,1)$ be an optimal solution of (\hat{P}_{kh}) . For k and h sufficiently small we have

$$\partial_{\nu}g_{kh}(\bar{\nu}_{kh},\bar{q}_{kh}) \leq -\bar{\eta}/2 < 0.$$

Proof. We use the representation of g', i.e. $\partial_{\nu}g(\nu,q) = \int_0^1 \langle Bq + \Delta u, z \rangle$ from (3.3). Then, the discretization error estimate (4.5) implies

$$\begin{aligned} \partial_{\nu}g_{kh}(\bar{\nu}_{kh},\bar{q}_{kh}) &\leq \partial_{\nu}g(\bar{\nu},\bar{q}) + c|\log k| \left(k+h^{2}\right) \\ &+ \left| \int_{0}^{1} \langle B\bar{q}_{kh} + \Delta u(\bar{\nu}_{kh},\bar{q}_{kh}), z(\bar{\nu}_{kh},\bar{q}_{kh}) \rangle - \int_{0}^{1} \langle B\bar{q} + \Delta \bar{u}, z(\bar{\nu},\bar{q}) \rangle \right|,\end{aligned}$$

where $z(\bar{\nu}, \bar{q})$ and $z(\bar{\nu}_{kh}, \bar{q}_{kh})$ denote the adjoint states with terminal values $\bar{u}(1) - u_d$ and $i_1S(\bar{\nu}_{kh}, \bar{q}_{kh}) - u_d$ and time transformations $\bar{\nu}$ and $\bar{\nu}_{kh}$. The convergence result Lemma 4.3 and complete continuity of the control-to-observation mapping, see Proposition A.1, imply $z(\bar{\nu}_{kh}, \bar{q}_{kh}) \rightarrow \bar{z}$ in W(0, 1). Hence, the result follows from the linearized Slater condition (3.4).

PROPOSITION 4.5. Let k and h be sufficiently small. Moreover, let $(\bar{\nu}, \bar{q})$ be the unique optimal solution of (\hat{P}) and let $(\bar{\nu}_{kh}, \bar{q}_{kh})$ be an optimal control of (\hat{P}_{kh}) . Then there exists a sequence $(\nu_{\tau})_{\tau>0}$ such that $(\nu_{\tau}, \bar{q}_{kh})$ are feasible for (\hat{P}) and

$$|\nu_{\tau} - \bar{\nu}_{kh}| \le c |\log k| (k+h^2).$$

Proof. Proceeding as in [5, Proposition 4.10] we set

$$\chi_{\tau} = (\nu_{\tau}, q_{\tau}) = (\bar{\nu}_{kh} + \tau, \bar{q}_{kh}).$$

for some $\tau \in (0, 1]$ to be determined later. Now, the proof is along the lines of the one of Proposition 4.2, interchanging the roles of $\bar{\chi} = (\bar{\nu}, \bar{q})$ and $\bar{\chi}_{kh} = (\bar{\nu}_{kh}, \bar{q}_{kh})$ and g and g_{kh} .

LEMMA 4.6. Let $(\bar{\nu}, \bar{q})$ be the unique optimal solution of problem (\hat{P}) such that Assumption 3.1 holds. Moreover, let $(\bar{\nu}_{kh}, \bar{q}_{kh}) \in \mathbb{R}_+ \times Q_{ad,\sigma}(0,1)$ be an optimal solution of (\hat{P}_{kh}) . Then, for k and h sufficiently small, we have

$$\left|\bar{\nu} - \bar{\nu}_{kh}\right| \le c \left(\sigma(k,h) + \left|\log k\right| (k+h^2)\right),$$

where c > 0 is independent of k and h. Moreover, there exists a unique Lagrange multiplier $\bar{\mu}_{kh} = \bar{\mu}_{kh}(\bar{q}_{kh}) > 0$ such that the optimality system is satisfied

(4.9)
$$\int_{0}^{1} 1 + \langle B\bar{q}_{kh}(t) + \Delta_{h}\bar{u}_{kh}(t), \bar{z}_{kh}(t) \rangle \, \mathrm{d}t = 0,$$

(4.10)
$$\int_0^1 \langle B^* \bar{z}_{kh}(t), q(t) - \bar{q}_{kh}(t) \rangle \, \mathrm{d}t \ge 0 \quad \text{for all } q \in Q_{ad,\sigma}(0,1),$$

(4.11)
$$G(\bar{u}_{kh}(1)) = 0,$$

where $\bar{u}_{kh} = S(\bar{\nu}_{kh}, \bar{q}_{kh})$ and $\bar{z}_{kh} \in X_{k,h}$ is the solution to the discrete adjoint equation

$$B(\bar{\nu}_{kh},\varphi_{kh},\bar{z}_{kh})=\bar{\mu}_{kh}(\bar{u}_{kh}(1)-u_d,\varphi_{kh}(1)),\quad\varphi_{kh}\in X_{k,h}.$$

Proof. Because the pair $(\nu_{\tau}, \bar{q}_{kh})$ is feasible for (\hat{P}) , we have

$$0 \le \nu_{\tau} - \bar{\nu} = \nu_{\tau} - \bar{\nu}_{kh} + \bar{\nu}_{kh} - \nu_{\gamma} + \nu_{\gamma} - \bar{\nu} \le \nu_{\tau} - \bar{\nu}_{kh} + \nu_{\gamma} - \bar{\nu},$$

where the last inequality follows from optimality of the pair $(\bar{\nu}_{kh}, \bar{q}_{kh})$ for (\hat{P}_{kh}) and feasibility of $(\nu_{\gamma}, q_{\gamma})$ for (\hat{P}_{kh}) . Hence,

$$\begin{aligned} |\bar{\nu}_{kh} - \bar{\nu}| &\leq |\bar{\nu}_{kh} - \nu_{\tau}| + \nu_{\tau} - \bar{\nu} \leq 2|\bar{\nu}_{kh} - \nu_{\tau}| + |\nu_{\gamma} - \bar{\nu}| \\ &\leq c \left(\sigma(k, h) + |\log k|(k + h^2)\right). \end{aligned}$$

where we have used Propositions 4.2 and 4.5 in the last step. Finally, the linearized Slater condition due to Proposition 4.4 yields the optimality conditions in qualified form as stated above.

REMARK 4.7. For each tuple $(\bar{\nu}_{kh}, \bar{q}_{kh}) \in \mathbb{R}_+ \times Q_{ad,\sigma}(0,1)$, there exists a unique Lagrange multiplier $\bar{\mu}_{kh}$. However, as the discrete control is not guaranteed to be unique, there might be different multipliers. Nevertheless, we can prove the a priori bound $\bar{\mu}_{kh} \leq 2/\bar{\eta}$ for k and h sufficiently small using the optimality conditions for (\hat{P}_{kh}) and Proposition 4.4.

4.2. Convergence of controls. Next, we prove convergence of the control variable based on the growth condition (3.14).

THEOREM 4.8. Let $(\bar{\nu}, \bar{q})$ be the global solution to (\hat{P}) such that Assumptions 3.1 and 3.2 hold. Moreover, let $(\bar{\nu}_{kh}, \bar{q}_{kh}) \in \mathbb{R}_+ \times Q_{ad,\sigma}(0,1)$ be an optimal solution of (\hat{P}_{kh}) . Then, we have $\bar{q}_{kh} \to \bar{q}$ in $L^1(I \times \Omega)$ and for k and h sufficiently small it holds

(4.12)
$$|\bar{\nu} - \bar{\nu}_{kh}| \le c \left(\sigma(k,h) + |\log k|(k+h^2)\right).$$

Proof. Let $\{(\bar{\nu}_{kh}, \bar{q}_{kh})\}$ be a sequence of globally optimal solutions to (\hat{P}_{kh}) that is guaranteed due to Lemma 4.3. The error estimate for the optimal times (4.12) is the assertion of Lemma 4.6. Since

$$|\nu_{\tau} - \bar{\nu}| \le |\nu_{\tau} - \bar{\nu}_{kh}| + |\bar{\nu}_{kh} - \bar{\nu}| \to 0,$$

and because the pair $(\nu_{\tau}, \bar{q}_{kh})$ is feasible for (\hat{P}) , we may use the growth condition from Theorem 3.8 to deduce

(4.13)
$$\frac{\bar{\nu}}{4}\Psi^{-1}\left(c_{0}\|\bar{q}_{kh}-\bar{q}\|_{L^{1}(I\times\omega)}\right)\|\bar{q}_{kh}-\bar{q}\|_{L^{1}(I\times\omega)}\leq\nu_{\tau}-\bar{\nu}.$$

Strict monotonicity and continuity of Ψ^{-1} finally imply $\bar{q}_{kh} \to \bar{q}$ in $L^1(I \times \Omega)$.

REMARK 4.9. If $\Psi(\varepsilon) = C\varepsilon^{\kappa}$, then in view of Remark 3.12 we obtain from (4.13) with similar arguments as in the proof of Lemma 4.6 the sub-optimal estimate

$$c \|\bar{q}_{kh} - \bar{q}\|_{L^1(I \times \omega)}^{1+1/\kappa} \le \nu_{\tau} - \bar{\nu} \le c \left(\sigma(k,h) + |\log k|(k+h^2)\right).$$

An improved estimate will be derived in the next section.

4.3. Improved error estimates for controls. Under certain conditions we will eventually provide an improved error estimate that is directly based on the structural condition (3.11). The required improved regularity in case of a distributed control is satisfied, if, e.g., $u_0 \in \mathcal{D}_{L^p}(-\Delta)$ with p > d/2, where we recall that d denotes the spatial dimension.

PROPOSITION 4.10. Adopt the assumptions of Theorem 4.8. Moreover, we assume that I_{σ} is the orthogonal projection onto $Q_{\sigma}(0,1)$ in $L^{2}(I \times \omega)$. In case of a distributed control, suppose in addition that $u_{0} \in (L^{p}, \mathcal{D}_{L^{p}}(-\Delta))_{1-1/s,s}$ for $s, p \in (1, \infty)$ such that d/(2p) + 1/s < 1. There is a constant c > 0 independent of k, h, $\bar{\nu}_{kh}$, and \bar{q}_{kh} such that

$$\Psi^{-1} \left(c_0 \| \bar{q} - \bar{q}_{kh} \|_{L^1(I \times \omega)} \right) \\ \leq c \left(| \bar{\nu} - \bar{\nu}_{kh} | + \| (\mathrm{Id} - \mathrm{I}_{\sigma}) B^* \hat{z}_{kh} \|_{L^{\infty}(I \times \omega)} + \| B^* \left(\hat{z}_{kh} - \hat{z} \right)) \|_{L^{\infty}(I \times \omega)} \right),$$

where $\hat{z} \in W(0,1)$ solves

$$-\partial_t \hat{z} - \bar{\nu}_{kh} \Delta \hat{z} = 0, \quad \hat{z}(1) = \bar{\mu} \left(\bar{u}_{kh}(1) - u_d \right),$$

and $\hat{z}_{kh} = (\bar{\mu}/\bar{\mu}_{kh})\bar{z}_{kh} \in X_{k,h}$ solves

(4.14)
$$B(\bar{\nu}_{kh},\varphi_{kh},\hat{z}_{kh}) = \bar{\mu}(\bar{u}_{kh}(1) - u_d,\varphi_{kh}(1)), \quad \varphi_{kh} \in X_{k,h}.$$

Proof. As in the proof of [34, Theorem 31], in (3.13) we set $q = \bar{q}_{kh}$ to obtain

$$(4.15) \quad \frac{\bar{\nu}}{2}\Psi^{-1}\left(c_0\|\bar{q}-\bar{q}_{kh}\|_{L^1(I\times\omega)}\right)\|\bar{q}-\bar{q}_{kh}\|_{L^1(I\times\omega)} \leq -\int_0^1 (B^*\bar{z},\bar{q}-\bar{q}_{kh})_{L^2(\omega)}\,\mathrm{d}t.$$

The optimality condition (4.10) with $q = I_{\sigma} \bar{q}$ multiplied by $\bar{\mu}/\bar{\mu}_{kh} > 0$ reads

(4.16)
$$0 \le \int_0^1 (B^* \hat{z}_{kh}, \mathbf{I}_\sigma \bar{q} - \bar{q}_{kh})_{L^2(\omega)} \, \mathrm{d}t,$$

where $\hat{z}_{kh} = (\bar{\mu}/\bar{\mu}_{kh})\bar{z}_{kh}$, i.e. \hat{z}_{kh} fulfills the same discrete adjoint equation as \bar{z}_{kh} but with multiplier $\bar{\mu}$ instead of $\bar{\mu}_{kh}$, as given in (4.14). Summation of (4.15) and (4.16) implies

$$\frac{\bar{\nu}}{2}\Psi^{-1}\left(c_{0}\|\bar{q}-\bar{q}_{kh}\|_{L^{1}(I\times\omega)}\right)\|\bar{q}-\bar{q}_{kh}\|_{L^{1}(I\times\omega)} \\
\leq \int_{0}^{1} \left(B^{*}\left(\hat{z}_{kh}-\bar{z}\right),\bar{q}-\bar{q}_{kh}\right)_{L^{2}(\omega)}\mathrm{d}t - \int_{0}^{1} \left(B^{*}\hat{z}_{kh},\bar{q}-\bar{q}_{kh}\right)_{L^{2}(\omega)}\mathrm{d}t \\
+ \int_{0}^{1} \left(B^{*}\hat{z}_{kh},\mathrm{I}_{\sigma}\bar{q}-\bar{q}_{kh}\right)_{L^{2}(\omega)}\mathrm{d}t \\
(4.17) \qquad = \int_{0}^{1} \left(B^{*}\left(\hat{z}_{kh}-\bar{z}\right),\bar{q}-\bar{q}_{kh}\right)_{L^{2}(\omega)}\mathrm{d}t + \int_{0}^{1} \left(B^{*}\hat{z}_{kh},\mathrm{I}_{\sigma}\bar{q}-\bar{q}\right)_{L^{2}(\omega)}\mathrm{d}t.$$

Concerning the first term of the right-hand side of (4.17), we have

(4.18)
$$\int_{0}^{1} (B^{*}(\hat{z}_{kh} - \bar{z}), \bar{q} - \bar{q}_{kh})_{L^{2}(\omega)} dt = \int_{0}^{1} (B^{*}(\hat{z}_{kh} - \hat{z}), \bar{q} - \bar{q}_{kh})_{L^{2}(\omega)} dt + \int_{0}^{1} (B^{*}(\hat{z} - \bar{z}), \bar{q} - \bar{q}_{kh})_{L^{2}(\omega)} dt + \int_{0}^{1} (B^{*}(\tilde{z} - \bar{z}), \bar{q} - \bar{q}_{kh})_{L^{2}(\omega)} dt,$$

where $\tilde{z} = z(\bar{\nu}, \bar{q}_{kh}) \in W(0, 1)$ is an additional adjoint state solving

$$-\partial_t \widetilde{z} - \overline{\nu} \Delta \widetilde{z} = 0, \quad \widetilde{z}(1) = \overline{\mu} \left(\widetilde{u}(1) - u_d \right), \quad \widetilde{u} = S(\overline{\nu}, \overline{q}_{kh})$$

Note that all adjoint states appearing above correspond to the same multiplier $\bar{\mu}$. For the first term on the right-hand side of (4.18), Hölder's inequality yields

$$\int_0^1 (B^* \left(\hat{z}_{kh} - \hat{z} \right), \bar{q} - \bar{q}_{kh})_{L^2(\omega)} \le \|B^* \left(\hat{z}_{kh} - \hat{z} \right)\|_{L^\infty(I \times \omega)} \|\bar{q} - \bar{q}_{kh}\|_{L^1(I \times \omega)}.$$

The second term on the right-hand side of (4.18) can be estimated using Proposition A.2 in case of purely time-dependent controls and Proposition A.3 in case of a distributed control as

$$\int_0^1 (B^* \left(\hat{z} - \widetilde{z} \right), \bar{q} - \bar{q}_{kh})_{L^2(\omega)} \le c |\bar{\nu}_{kh} - \bar{\nu}| \|\bar{q} - \bar{q}_{kh}\|_{L^1(I \times \omega)}.$$

The third term on the right-hand side of (4.18) is less than or equal to zero, because of affine linearity of $i_1S(\bar{\nu}, q)$ with respect to q which implies

$$\int_{0}^{1} (B^{*} (\tilde{z} - \bar{z}), \bar{q} - \bar{q}_{kh})_{L^{2}(\omega)} dt$$

= $\bar{\mu} (\left(i_{1} (\partial_{t} - \bar{\nu}\Delta)^{-1}\right)^{*} (\tilde{u}(1) - \bar{u}(1)), B(\bar{q} - \bar{q}_{kh}))_{L^{2}} = -\bar{\mu} \|\bar{u}(1) - \tilde{u}(1)\|_{L^{2}}^{2}$

where $(\partial_t - \bar{\nu}\Delta)^{-1}$ denotes the solution operator to the linear heat-equation with homogeneous initial data. Since I_{σ} is the $L^2(I \times \omega)$ -projection onto $Q_{\sigma}(0,1)$ for the last term of the right-hand side of (4.17) we obtain

$$\int_0^1 (B^* \hat{z}_{kh}, \mathbf{I}_{\sigma} \bar{q} - \bar{q})_{L^2(\omega)} \, \mathrm{d}t = \int_0^1 ((\mathrm{Id} - \mathbf{I}_{\sigma}) B^* \hat{z}_{kh}, \bar{q}_{kh} - \bar{q})_{L^2(\omega)} \, \mathrm{d}t.$$

In summary, we arrive at

$$\frac{\bar{\nu}}{2}\Psi^{-1}\left(c_{0}\|\bar{q}-\bar{q}_{kh}\|_{L^{1}(I\times\omega)}\right)\|\bar{q}-\bar{q}_{kh}\|_{L^{1}(I\times\omega)} \leq c\left(|\bar{\nu}_{kh}-\bar{\nu}|\right) \\
+\|(\mathrm{Id}-\mathrm{I}_{\sigma})B^{*}\hat{z}_{kh}\|_{L^{\infty}(I\times\omega)} + \|B^{*}\left(\hat{z}_{kh}-\hat{z}\right)\|_{L^{\infty}(I\times\omega)}\right)\|\bar{q}-\bar{q}_{kh}\|_{L^{1}(I\times\omega)}.$$

Last, dividing by $\|\bar{q} - \bar{q}_{kh}\|_{L^1(I \times \omega)}$ yields the desired estimate.

4.4. Concrete control discretization schemes. Before we apply the general results of the preceding subsections, we will verify the equivalence of a semi-variational and an explicit discretization of the controls. To this end, let $Q_h \subseteq Q$ be a finite dimensional subspace. In the following we consider for given Q_h the two choices of the control space $Q_{\sigma}(0, 1)$: the discrete control space $Q_{\sigma}(0, 1) = Q_{kh}(0, 1)$, where

(4.19)
$$Q_{kh}(0,1) = \{ v \in Q(0,1) \colon v |_{I_m} \in \mathcal{P}_0(I_m;Q_h), \ m = 1, 2, \dots, M \},\$$

and the semi-variational control space $Q_{\sigma}(0,1) = L^2(I;Q_h)$. Additionally, let Π_k denote the L^2 -projection onto the piecewise constant functions in time. The problem (\hat{P}_{kh}) posed with $Q_{\sigma}(0,1) = Q_{kh}(0,1)$ is equivalent to (\hat{P}_{kh}) with $Q_{\sigma}(0,1) = L^2(I;Q_h)$ in the following sense.

PROPOSITION 4.11. If $(\bar{\nu}_{kh}, \bar{q}_{kh})$ is an optimal solution to (\hat{P}_{kh}) with $Q_{\sigma}(0,1) = Q_{kh}(0,1)$ then $(\bar{\nu}_{kh}, \bar{q}_{kh})$ is also optimal for (\hat{P}_{kh}) with $Q_{\sigma}(0,1) = L^2(I;Q_h)$. Conversely, if $(\bar{\nu}_{kh}^{v}, \bar{q}_{kh}^{v})$ is an optimal solution to (\hat{P}_{kh}) with $Q_{\sigma}(0,1) = L^2(I;Q_h)$, then $(\bar{\nu}_{kh}^{v}, \Pi_k \bar{q}_{kh}^{v})$ is also optimal for (\hat{P}_{kh}) with $Q_{\sigma}(0,1) = Q_{kh}(0,1)$.

Proof. First, since the variational admissible set $L^2(I; Q_h) \cap Q_{ad}(0, 1)$ is larger than the fully discrete one $Q_{kh}(0, 1) \cap Q_{ad}(0, 1)$, we immediately obtain $\bar{\nu}_{kh}^{\mathsf{v}} \leq \bar{\nu}_{kh}$ for the optimal times. Clearly, $\Pi_k \bar{q}_{kh}^{\mathsf{v}} \in Q_{kh}(0, 1) \cap Q_{ad}(0, 1)$ by the fact that Π_k can be computed explicitly on every interval I_m as the interval mean. In addition, by the orthogonality-properties of the L^2 -projection Π_k and the definition of the state equation (4.1), $(\bar{\nu}_{kh}^{\mathsf{v}}, \Pi_k \bar{q}_{kh}^{\mathsf{v}})$ has the same associated discrete state as $(\bar{\nu}_{kh}^{\mathsf{v}}, \bar{q}_{kh}^{\mathsf{v}})$, which directly implies that $g_{kh}(\bar{\nu}_{kh}^{\mathsf{v}}, \Pi_k \bar{q}_{kh}^{\mathsf{v}}) \leq 0$. Thus, $(\bar{\nu}_{kh}^{\mathsf{v}}, \Pi_k \bar{q}_{kh}^{\mathsf{v}})$ is feasible for (\hat{P}_{kh}) with $Q_{\sigma}(0, 1) = Q_{kh}(0, 1)$ and therefore $\bar{\nu}_{kh} \leq \bar{\nu}_{kh}^{\mathsf{v}}$. Hence, both problems have the same optimal time $\bar{\nu}_{kh} = \bar{\nu}_{kh}^{\mathsf{v}}$. Consequently, the optimal controls of both problems are given by all controls $q \in Q_{ad,\sigma}(0, 1)$ such that $g_{kh}(\bar{\nu}_{kh}, q) \leq 0$, with $Q_{\sigma}(0, 1) = Q_{kh}(0, 1) = L^2(I; Q_h)$, respectively. A similar argument as before yields the relation between the optimal controls as claimed.

As we are interested in explicit rates of convergence, for the following considerations we assume that $\Psi(\varepsilon) = C\varepsilon^{\kappa}$ in (3.11). The proceeding results hold for a general function Ψ satisfying (3.11) with obvious modifications.

4.4.1. Purely time-dependent controls. In case of purely time-dependent controls we immediately derive an error estimate (that is optimal if $\kappa = 1$) using the $L^{\infty}(I; L^2)$ discretization error estimate for the variational control discretization. Note that besides theoretical advantages purely time-dependent controls are also interesting in practice as distributed controls are typically difficult to implement.

THEOREM 4.12 (Parameter control, variational). Adopt the assumptions of Theorem 4.8 and let (3.11) hold with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$. Additionally, suppose purely timedependent controls and let $(\bar{\nu}_{kh}, \bar{q}_{kh})$ be an optimal solution of (\hat{P}_{kh}) with $Q_{\sigma}(0, 1) = L^2(I, \mathbb{R}^{N_c})$. Then there is a constant c > 0 such that

$$|\bar{\nu} - \bar{\nu}_{kh}| + \|\bar{q} - \bar{q}_{kh}\|_{L^1(I \times \omega)}^{1/\kappa} \le c |\log k| (k+h^2).$$

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Proof. This follows from Proposition 4.10, since in case of purely time-dependent control we may use the $L^{\infty}(I; L^2)$ discretization error estimate, see Lemma A.4, for the state and adjoint state equation to obtain

$$\begin{aligned} \|B^* \left(\hat{z}_{kh} - \hat{z} \right)\|_{L^{\infty}(I \times \omega)} &= \operatorname{ess\,sup}_{i \in \{1, \dots, N_c\}} \max_{i \in \{1, \dots, N_c\}} |(e_i, \hat{z}_{kh}(t) - \hat{z}(t))| \\ &\leq c \|\hat{z}_{kh} - \hat{z}\|_{L^{\infty}(I:L^2)} \leq c |\log k| (k+h^2). \end{aligned}$$

In addition, $\sigma(k, h) = 0$ as we do not explicitly discretize the control variable. The remaining estimate for $\bar{\nu}$ is proved in Lemma 4.6.

Next, we consider an explicitly discretized control variable. Using Proposition 4.11 with $Q_h = \mathbb{R}^{N_c}$, we immediately obtain the following result.

COROLLARY 4.13 (Parameter control, discrete). The result of Theorem 4.12 remains valid for piecewise constant controls $Q_{\sigma}(0,1) = Q_{kh}(0,1)$ with $Q_h = \mathbb{R}^{N_c}$ under the same assumptions.

4.4.2. Distributed control with variational control discretization. Next, we discuss the case of a distributed control, i.e. $\omega \subset \Omega$. In order to apply Proposition 4.10 we require pointwise error estimates for the adjoint state equation. For simplicity, we only consider the particular case that the control domain ω has a strict distance to the boundary $\partial \Omega$ of the spatial domain and smooth initial and desired states. Moreover, assume in the remaining part of this section that the spatial mesh is quasi-uniform. Based on pointwise best approximations results from [24] we can obtain the following error estimate. For its proof we refer to [2, Sections 5.5.3, 5.5.4].

PROPOSITION 4.14 ([2, Proposition 5.41]). Let $\overline{\omega} \subset \Omega$. Suppose that $u_0, u_d \in \mathcal{D}_{L^{\infty}}(-\Delta)$. Then there exists a constant c > 0, independent of k, h, \hat{z}_{kh} , and \hat{z} , such that

$$\|B^*(\hat{z}_{kh} - \hat{z})\|_{L^{\infty}(I \times \omega)} \le c |\log k|^4 |\log h|^7 (k + h^2).$$

We directly infer the following error estimate for the variational control discretization.

THEOREM 4.15 (Variational discretization). Adopt the assumptions of Theorem 4.8 and let (3.11) hold with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$. Moreover, suppose the variational control discretization, i.e. $Q_{\sigma}(0,1) = Q(0,1)$. In addition, assume $\overline{\omega} \subset \Omega$ as well as $u_0, u_d \in \mathcal{D}_{L^{\infty}}(-\Delta)$. Then there is a constant c > 0, independent of k, h, $\overline{\nu}_{kh}$, and \overline{q}_{kh} , such that

$$|\bar{\nu} - \bar{\nu}_{kh}| + \|\bar{q} - \bar{q}_{kh}\|_{L^1(I \times \omega)}^{1/\kappa} \le c |\log k|^4 |\log h|^7 (k + h^2).$$

Proof. This result follows from Theorem 4.8 and Propositions 4.10 and 4.14, since for the variational control discretization we have $I_{\sigma} = Id$ and $\sigma(k, h) = 0$.

4.4.3. Distributed control with cellwise constant control discretization. Last, we consider the discretization of the control by cellwise constant functions in space. Recall that $\sigma(k,h)$ denotes the projection error onto $Q_{\sigma}(0,1)$ measured $L^2(I; H^{-1})$; see (4.2). Since the control variable has a bang-bang structure, we cannot expect order k of convergence in L^2 in time. We therefore first consider a semivariational control discretization and obtain the fully discrete result using Proposition 4.11. Let the discrete space of controls be defined as follows

$$Q_h = \left\{ v \in L^2(\omega) \colon v |_K \in \mathcal{P}_0(K) \text{ for all } K \in \mathcal{T}_h^{\omega} \right\}, \quad Q_\sigma(0,1) = L^2(I;Q_h).$$

Hence, the controls are explicitly discretized in space but not explicitly discretized in time, which is equivalent to the discretization by piecewise and cellwise constant functions. Let $\Pi_{h,0}$ denote the $L^2(\omega)$ -projection onto the cellwise constant functions. Moreover, for almost every $t \in [0, 1]$ we set

$$\mathcal{S}_{h,t} \coloneqq \mathcal{T}_h^{\omega} \setminus \{ K \in \mathcal{T}_h^{\omega} : \bar{q}(t) |_K \equiv q_a \text{ or } \bar{q}(t) |_K \equiv q_b \}$$

We first establish error estimates for $\sigma(k, h)$ with $I_{\sigma} = \prod_{h,0}$.

PROPOSITION 4.16. Suppose there are functions $\delta_h \in L^1(I)$, h > 0, and a constant c > 0 such that

(4.20)
$$\sum_{K \in \mathcal{S}_{h,t}} |K| \le \delta_h(t), \quad a.e. \ t \in [0,1], \quad h > 0,$$

and $\|\delta_h\|_{L^1(I)} \leq ch$ for all h > 0. Then the estimate

(4.21)
$$\|B(\Pi_{h,0}\bar{q}-\bar{q})\|_{L^2(I;H^{-1})} \le ch^{3/2},$$

holds with a constant c > 0 not depending on h.

Proof. Since $\Pi_{h,0}$ is a projection, for any $v \in H^1$ and $K \in \mathcal{T}_h^{\omega}$ we have

$$(\Pi_{h,0}\bar{q}(t) - \bar{q}(t), v)_{L^{2}(K)} \le ch \|\Pi_{h,0}\bar{q}(t) - \bar{q}(t)\|_{L^{2}(K)} \|\nabla v\|_{L^{2}(K)}.$$

Using Hölder's inequality and the supposition (4.20) yields (4.21).

We have the following sufficient condition for (4.20), which is proved along the lines of the proof of [9, Theorem 4.4].

PROPOSITION 4.17. If $B^* \overline{z} \in L^1(I; C^1(\overline{\omega}))$ and (3.11) holds with $\Psi(\varepsilon) = C\varepsilon$, then (4.20) is valid.

Finally, we provide error estimates for cellwise constant control discretization.

THEOREM 4.18 (Cellwise constant controls). Adopt the assumptions of Theorem 4.8 and let (3.11) hold with $\Psi(\varepsilon) = C\varepsilon^{\kappa}$. Moreover, suppose the variational in time and cellwise constant control discretization in space, i.e. $Q_{\sigma}(0,1) = L^2(I;Q_h)$. In addition, assume $\overline{\omega} \subset \Omega$, $u_0, u_d \in \mathcal{D}_{L^{\infty}}(-\Delta)$, and that (4.20) is satisfied. There is a c > 0 not depending on k, h, $\overline{\nu}_{kh}$, and \overline{q}_{kh} such that

$$\begin{aligned} |\bar{\nu} - \bar{\nu}_{kh}| &\leq c |\log k| (k+h^{3/2}), \\ \|\bar{q} - \bar{q}_{kh}\|_{L^1(I \times \omega)}^{1/\kappa} &\leq c |\log k|^4 |\log h|^7 (k+h). \end{aligned}$$

Proof. The error estimate Proposition 4.14 and stability of Id $-\Pi_{h,0}$ in L^{∞} yield

$$\|(\mathrm{Id} - \Pi_{h,0})B^*\hat{z}_{kh}\|_{L^{\infty}(I \times \omega)} \le c|\log k|^4 |\log h|^7 (k+h^2) + \|(\mathrm{Id} - \Pi_{h,0})B^*\hat{z}\|_{L^{\infty}(I \times \omega)}$$

Moreover, employing elliptic regularity with some p > d, we have the estimate

$$\|(\mathrm{Id} - \Pi_{h,0})B^*\hat{z}\|_{L^{\infty}(I \times \omega)} \le ch\|\hat{z}\|_{L^{\infty}(I;W^{2,p}(\omega))} \le ch\|\hat{z}\|_{L^{\infty}(I;\mathcal{D}_{L^p}(-\Delta))} \le ch.$$

Hence, using Theorem 4.8, Propositions 4.10 and 4.14 as well as the estimates for σ from Proposition 4.16 we infer the desired estimate.

Using Proposition 4.11, we immediately obtain the following result.

COROLLARY 4.19 (Piecewise and cellwise constant controls). The result of Theorem 4.18 remains valid for $Q_{\sigma}(0,1) = Q_{kh}(0,1)$ under the same assumptions.

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5. Numerical examples. We verify the theoretical results by numerical examples. In order to solve the optimization problem (\hat{P}) , we employ the equivalence of time- and distance optimal control problems summarized in Appendix B (see also [3]), and solve a sequence of optimization problems with a fixed time. The resulting convex sub-problems for a fixed time are solved by an accelerated conditional gradient method. In an outer loop the optimal time is determined by a Newton method. For further details we refer to [3]. The computations are performed in MATLAB.

5.1. Example with purely time-dependent control. We take the example from [5, Section 5.2] with purely time-dependent controls for fixed spatially dependent functions but without control costs in the objective functional. Let

$$\begin{aligned} \Omega &= (0,1)^2, \quad \omega_1 = (0,0.5) \times (0,1), \quad \omega_2 = (0.5,1) \times (0,0.5), \\ B &: \mathbb{R}^2 \to L^2(\Omega), \quad Bq = q_1 \chi_{\omega_1} + q_2 \chi_{\omega_2}, \\ Q_{ad}(0,1) &= \{q \in L^2(I; \mathbb{R}^2): -1.5 \le q \le 0\}, \\ u_0(x) &= 4 \sin(\pi x_1^2) \sin(\pi x_2^3), \quad u_d(x) = 0, \quad \delta_0 = 1/10, \end{aligned}$$

where χ_{ω_1} and χ_{ω_2} denote the characteristic functions on ω_1 and ω_2 . The spatial mesh is chosen such that the boundaries of ω_1 and ω_2 coincide with edges of the mesh. We discretize the control by piecewise constant functions in time.



FIG. 5.1. Discretization error for Example 5.1 with piecewise constant control discretization and refinement of the time interval for N = 4225 nodes (left) and refinement of the spatial discretization for M = 640 time steps (right). The reference solution is calculated for N = 16641 and M = 1280.



FIG. 5.2. The switching function $B^*\bar{z}$ from Example 5.1 near zero.

Since the exact solution is unknown, we calculate a numerical solution on a sufficiently fine grid. In accordance with Corollary 4.13 (provided that (3.11) holds with

 $\Psi(\varepsilon) = C\varepsilon$, see also the plot of the switching function in Figure 5.2 and the numerical test in Figure 5.5), we observe linear convergence with respect to k and quadratic order of convergence in h for all variables; see Figure 5.1.

5.2. Example with distributed control on subdomain. Next, we consider the example from [5, Section 5.3] with distributed control on the subset $\omega = (0, 0.75)^2$ of the domain $\Omega = (0, 1)^2$. As before we compare to a reference solution obtained numerically on a fine grid. The control bounds are $q_a = -5$, $q_b = 0$, and the data is

$$u_d(x) = -2\min\{x_1, 1 - x_1, x_2, 1 - x_2\}, \quad \delta_0 = 1/10$$

$$u_0(x) = 4\sin(\pi x_1^2)\sin(\pi x_2)^3.$$

We consider the piecewise and cellwise constant discretization for the control variable. As in the first example we observe full order of convergence with respect to the terminal time. However, we do not have full order convergence for the control variable. From Figure 5.3 we approximately estimate the rate $k^{1/2}$ and h, respectively, for the control variable. Numerically evaluating the condition (3.11) we observe that the



FIG. 5.3. Discretization error for Example 5.2 with piecewise and cellwise constant control discretization and refinement of the time interval for N = 4225 nodes (left) and refinement of the spatial discretization for M = 320 time steps (right). The reference solution is calculated for N = 16641 and M = 640.

structural assumption is not satisfied with $\kappa = 1$ in this example; see Figure 5.5 (cf. also Figure 5.4 for a plot of the switching function). For this reason, we cannot expect the rate k for the control variable employing Theorem 4.18. In Example 5.1 we observe linear decrease while in Example 5.2 it is hard to determine the rate of decrease; see Figure 5.5.

Appendix A. Regularity results and discretization error estimates.

PROPOSITION A.1 ([2, Proposition A.19]). Let s > 2 and $u_0 \in L^2$. The mapping $(\nu, q) \mapsto S(\nu, q)$ is completely continuous from $\mathbb{R} \times L^s(I \times \omega)$ into $C([0, 1]; L^2)$.

For the proof of Proposition 4.10 we require the following Lipschitz-type estimate of the solution to the state equation with respect to the time transformation.

PROPOSITION A.2. Let $\nu_{\max} > \nu_{\min} > 0$. There is c > 0 such that for any $u_0 \in L^2$, $f \in L^2(I; H^{-1})$, and $\nu_1, \nu_2 \in [\nu_{\min}, \nu_{\max}]$ the solutions to the state equation $u(\nu_1) = u(\nu_1, u_0, f)$ and $u(\nu_2) = u(\nu_2, u_0, f)$ satisfy the estimate

$$\|u(\nu_1) - u(\nu_2)\|_{C([0,1];L^2)} \le c|\nu_1 - \nu_2| \left(\|f\|_{L^2(I;H^{-1})} + \|u_0\|_{L^2} \right),$$



FIG. 5.4. Snapshots of switching function $B^*\bar{z}$ from Example 5.2 (with color scale adapted to values below 10^{-6}).



FIG. 5.5. Numerical verification of structural assumption on adjoint state (3.11) for Example 5.1 (left) and Example 5.2 (right).

where c > 0 is independent of ν , f, and u_0 .

Proof. Set $u_1 = u(\nu_1)$ and $u_2 = u(\nu_2)$. Then the difference $w = u_1 - u_2$ satisfies

 $\partial_t w - \nu_1 \Delta w = (\nu_1 - \nu_2) (\Delta u_2 + f), \quad w(0) = 0.$

Hence, standard energy estimates lead to

$$||w||_{H^{1}(I;H^{-1})\cap L^{2}(I;H^{1})} \leq c|\nu_{1}-\nu_{2}|||-\Delta u_{2}+f||_{L^{2}(I;H^{-1})}$$
$$\leq c|\nu_{1}-\nu_{2}|\left(||f||_{L^{2}(I;H^{-1})}+||u_{0}||_{L^{2}}\right).$$

Last, the assertion follows from $H^1(I; H^{-1}) \cap L^2(I; H^1) \hookrightarrow C([0, 1]; L^2)$.

PROPOSITION A.3. Let $\nu_{\max} > \nu_{\min} > 0$ and $s, p \in (1, \infty)$ such that d/(2p) + 1/s < 1. There is c > 0 such that for any $u_0 \in (L^p, \mathcal{D}_{L^p}(-\Delta))_{1-1/s,s}$, $f \in L^s(I; L^p)$, and $\nu_1, \nu_2 \in [\nu_{\min}, \nu_{\max}]$ the solutions to the state equation $u(\nu_1) = u(\nu_1, u_0, f)$ and $u(\nu_2) = u(\nu_2, u_0, f)$ satisfy the estimate

$$\|u(\nu_1) - u(\nu_2)\|_{L^{\infty}(I \times \Omega)} \le c|\nu_1 - \nu_2| \left(\|f\|_{L^s(I;L^p)} + \|u_0\|_{(L^p,\mathcal{D}_{L^p}(-\Delta))_{1-1/s,s}} \right),$$

where c > 0 is independent of ν , f, and u_0 .

Proof. Maximal parabolic regularity of $-\Delta$ on L^p , see, e.g., [14, Theorem 2.9 b)], yields that the solution $u = u(\nu, f, u_0)$ satisfies the estimate

$$\|u\|_{W^{1,s}(I;L^p)\cap L^s(I;\mathcal{D}_{L^p}(-\Delta))} \le c\left(\|f\|_{L^s(I;L^p)} + \|u_0\|_{(L^p,\mathcal{D}_{L^p}(-\Delta))_{1-1/s,s}}\right).$$

Moreover, continuity of $\nu \mapsto (\partial_t - \nu \Delta)^{-1}$, $\nu > 0$, as well as compactness of $[\nu_{\min}, \nu_{\max}]$ imply that the constant in the estimate above can be chosen uniformly with respect to ν . Set $u_1 = u(\nu_1)$ and $u_2 = u(\nu_2)$. Then the difference $w = u_1 - u_2$ satisfies

$$\partial_t w - \nu_1 \Delta w = (\nu_1 - \nu_2) (\Delta u_2 + f), \quad w(0) = 0.$$

Hence,

$$\begin{aligned} \|w\|_{W^{1,s}(I;L^p)\cap L^s(I;\mathcal{D}_{L^p}(-\Delta))} &\leq c|\nu_1-\nu_2|\|-\Delta u_2+f\|_{L^s(I;L^p)}\\ &\leq c|\nu_1-\nu_2|\left(\|f\|_{L^s(I;L^p)}+\|u_0\|_{(L^p,\mathcal{D}_{L^p}(-\Delta))_{1-1/s,s}}\right).\end{aligned}$$

Finally, the assertion follows from the embedding

$$W^{1,s}(I;L^p) \cap L^s(I;\mathcal{D}_{L^p}(-\Delta)) \hookrightarrow C(\overline{I \times \Omega});$$

see the proof of [14, Theorem 3.1].

LEMMA A.4 ([5, Lemma B.2]). Let $\nu \in \mathbb{R}_+$ and $f \in L^{\infty}((0,1); L^2)$. For the solution $u = u(\nu, f)$ to the state equation with right-hand side f and the discrete solution $u_{kh} = u_{kh}(\nu, f)$ to equation (4.1) with right-hand side f it holds

(A.1)
$$\|u - u_{kh}\|_{L^{\infty}(I;L^2)} \le c |\log k| (k + h^2) ((1 + \nu) \|f\|_{L^{\infty}(I;L^2)} + \nu^{-1} \|u_0\|_{L^2}),$$

(A.2)
$$\|u - u_{kh}\|_{L^{\infty}(I;L^2)} \le c |\log k| (k + h^2) (1 + \nu) (\|f\|_{L^{\infty}(I;L^2)} + \|\Delta u_0\|_{L^2}),$$

where the constant c is independent of ν , k, h, f, u_0 , and u.

PROPOSITION A.5. Let $\nu_{\max} \in \mathbb{R}_+$, $q \in Q_{ad}(0,1)$, and $u_0 \in L^2$. Then

$$\lim_{k,h\to 0} \sup_{\nu \in (0,\nu_{\max})} \|i_1 S_{kh}(\nu,q) - i_1 S(\nu,q)\|_{L^2} = 0.$$

Proof. We abbreviate $u_{kh} = S_{kh}(\nu, q)$ and $u = S(\nu, q)$. Consider first the case q = 0. Let $\varepsilon > 0$ be given. Due to density of H^2 in L^2 there exists $u_{0,\varepsilon} \in H^2$ such that $||u_0 - u_{0,\varepsilon}|| \leq \varepsilon$. Let u_{ε} and $u_{kh,\varepsilon}$ denote the corresponding continuous and discrete solutions to the state equation with initial value $u_{0,\varepsilon}$. Using the stability estimates [5, Proposition 4.1] and [5, Proposition A.1] as well as the discretization error estimate (A.2) we find

$$\begin{aligned} \|u_{kh}(1) - u(1)\|_{L^2} &\leq \|u_{kh}(1) - u_{kh,\varepsilon}(1)\|_{L^2} + \|u_{kh,\varepsilon}(1) - u_{\varepsilon}(1)\|_{L^2} + \|u_{\varepsilon}(1) - u(1)\|_{L^2} \\ &\leq c \|\Pi_h (u_0 - u_{0,\varepsilon})\|_{L^2} + c |\log k| (k+h^2) \|\Delta u_{0,\varepsilon}\|_{L^2} + c \|u_{0,\varepsilon} - u_0\|_{L^2}, \end{aligned}$$

with a constant c independent of k, h, ν , and ε . Therefore, employing stability of the projection Π_h in L^2 , for k, h > 0 sufficiently small such that $|\log k|(k+h^2)||\Delta u_{0,\varepsilon}||_{L^2} \le \varepsilon$ we obtain the estimate $||u_{kh}(1) - u(1)||_{L^2} \le c\varepsilon$. In the case $u_0 = 0$, we can directly apply the discretization error estimate (A.1).

Appendix B. Algorithmic aspects. In order to solve the optimization problem (\hat{P}) one could add a regularization term to the objective functional (cf. also [2, Section 5.5]) and solve the auxiliary problem for a decreasing sequence of regularization parameters equipped with a path-following strategy. However, for small α the resulting problems become computationally very expensive. In this section we describe an alternative approach based on an equivalent reformulation. For further details we refer to [3].

B.1. Equivalence of time and distance optimal controls. For any $\delta \geq 0$ we consider the *perturbed time-optimal control problem*

(P_{$$\delta$$}) Minimize T subject to $T \in \mathbb{R}_+, q \in Q_{ad}(0,T),$
 $\|u_q(T) - u_d\|_{L^2} \leq \delta_0 + \delta.$

Moreover, for fixed T > 0 we consider the minimal distance control problem

(P_T) Minimize
$$||u_q(T) - u_d||_{L^2} - \delta_0$$
 subject to $q \in Q_{ad}(0,T)$.

Note that (P_T) is a nonlinear and nonconvex optimization problem subject to control as well as state constraints, whereas (P_T) is a convex problem subject to control bounds only.

We define the value functions $T: [0, \infty) \to [0, \infty]$ and $\delta: [0, \infty) \to [0, \infty)$ as

 $T(\delta) = \inf (P_{\delta})$ and $\delta(T) = \inf (P_T)$.

From boundedness of Q_{ad} , linearity of the control-to-state mapping (for fixed T > 0), and weak lower semicontinuity of the norm function, we immediately infer that the value function $\delta(\cdot)$ is well-defined. Furthermore, under Assumption 2.3, standard arguments lead to well-posedness of $T(\cdot)$.

The problems (P_{δ}) and (P_T) are connected to each other in the following sense – provided that $T(\cdot)$ is left continuous which we will assume throughout the remaining article. If $T \in (0, T(0)]$ and $q \in Q_{ad}(0, T)$ is distance-optimal for (P_T) , then (T, q) is also time-optimal for $(P_{\delta(T)})$. Conversely, if $\delta \in [0, \delta^{\bullet}]$ with $\delta^{\bullet} = ||u_0 - u_d||_{L^2} - \delta_0$ and $(T, q) \in \mathbb{R}_+ \times Q_{ad}(0, T)$ is time-optimal for (P_{δ}) , then q is also distance-optimal for (δ_T) .

In view of the relation between (P_{δ}) and (P_T) , we are interested in finding a root of the value function $\delta(\cdot)$ to solve the time-optimal control problem (P). This leads to a bi-level optimization problem: In the outer loop we search for a root of $\delta(\cdot)$ and the inner loop determines for each given T a control such that the associated state has minimal distance to the target set.

B.2. Newton method for the outer loop. Similarly as in Section 3, we transform the minimal distance control problem (P_T) to the reference time interval (0, 1). For fixed $\nu \in \mathbb{R}_+$, let $\nu \mapsto \bar{q}(\nu)$ be the (possibly) multi-valued function

(B.1)
$$\bar{q}(\nu) = \underset{q \in Q_{ad}(0,1)}{\operatorname{argmin}} \|i_1 S(\nu, q) - u_d\|_{L^2}.$$

We consider the associated value function $\delta \colon \mathbb{R}_+ \to \mathbb{R}$ defined by

$$\delta(\nu) = \|i_1 S(\nu, q) - u_d\|_{L^2} - \delta_0, \quad q \in \bar{q}(\nu).$$

Formally differentiating the value function yields

(B.2)
$$\delta'(\nu) = \int_0^1 \langle Bq + \Delta u, \bar{z} \rangle \, \mathrm{d}t, \quad q \in \bar{q}(\nu),$$

where $u = S(\nu, q)$ and $\bar{z} \in W(0, 1)$ satisfies

(B.3)
$$-\partial_t \bar{z} - \nu \Delta \bar{z} = 0, \quad \bar{z}(1) = \left(\bar{u}(1) - u_d\right) / \|\bar{u}(1) - u_d\|_{L^2}.$$

The resulting Newton method is summarized in Algorithm B.1. We emphasize that given a solution $q \in \bar{q}(\nu)$, the derivative $\delta'(\nu)$ can be efficiently computed. Indeed, the

required variables for the evaluation of (B.2) will typically be directly available from the optimization of the inner loop. For this reason, one step of the Newton method has approximately the same computational costs as one step of, e.g., the bisection method.

Algorithm B.1 Newton method for solution of minimal distance problem

1: Choose $\nu_0 > 0$ 2: for $n = 0, ..., n_{\max}$ do 3: Calculate $q_n = \overline{q}(\nu_n)$ using Algorithm B.2 and $u_n = S(\nu_n, q_n)$ 4: if $\delta(\nu_n) < \varepsilon_{tol}$ then 5: return 6: end if 7: Evaluate $\delta'(\nu_n)$ using (B.2) 8: Set $\nu_{n+1} = \nu_n - \delta(\nu_n)\delta'(\nu_n)^{-1}$ 9: end for

B.3. Conditional gradient method for the inner optimization. For the algorithmic solution of the inner problem, i.e. the determination of $\bar{q}(\nu)$ in (B.1), we employ the conditional gradient method; see, e.g., [15]. We abbreviate

$$f(q) = \|i_1 S(\nu, q) - u_d\|_{L^2}$$

neglecting the ν dependence for a moment. Differentiability of the control-to-state mapping yields

$$f'(q)^* = \nu B^* z,$$

where $z \in W(0, 1)$ solves (B.3) with $u = S(\nu, q)$. Given $q_n \in Q_{ad}(0, 1)$, we take

(B.4)
$$q_{n+1/2} = \begin{cases} q_a, & \text{if } B^* z_n > 0, \\ q_b, & \text{if } B^* z_n < 0, \\ (q_a + q_b)/2, & \text{else}, \end{cases}$$

almost everywhere. The next iterate q_{n+1} is defined by the optimal convex combination of q_n and $q_{n+1/2}$, i.e.

(B.5)
$$\lambda_n = \operatorname*{argmin}_{0 \le \lambda \le 1} f((1-\lambda)q_n + \lambda q_{n+1/2}).$$

This expression can be analytically determined, employing the fact that $q \mapsto S(\nu, q)$ is affine linear. Using convexity of f and the definition of $q_{n+1/2}$, we immediately obtain the following a posteriori error estimator

$$0 \le f(q_n) - f(\bar{q}) \le f'(q_n)(q_n - \bar{q}) \le \max_{q \in Q_{ad}(0,1)} f'(q_n)(q_n - q) = f'(q_n)(q_n - q_{n+1/2}).$$

The expression on the right-hand side can be efficiently evaluated using the adjoint representation and serves as a termination criterion for the conditional gradient method. The algorithm for the inner optimization is summarized in Algorithm B.2.

Under a structural assumption on the adjoint state such as (3.11) with $\Psi(\varepsilon) = C\varepsilon$ and purely time-dependent controls the conditional gradient method is known to converge q-linearly; cf. [15, Theorem 3.1 (iii)]. However, in general only sublinear convergence is guaranteed; see [15, Theorem 3.1 (i)]. For this reason, we have implemented an acceleration strategy, where instead of (B.5) we use the best convex combination of all iterates $q_{j+1/2}$, j = 0, 1, 2, ..., n + 1, with $q_{0+1/2} \coloneqq q_0$. Algorithm B.2 Conditional gradient method for solution of (B.1)

1: Let $\nu > 0$ be given. Choose $q_0 \in Q_{ad}(0, 1)$

2: for $n = 0, ..., n_{\max}$ do

- 3: Calculate $u_n = S(\nu, q_n)$ and z_n
- 4: Choose $q_{n+1/2}$ as in (B.4)
- 5: **if** $f'(q_n)(q_n q_{n+1/2}) < \varepsilon_{\text{tol}}$ **then**
- 6: return
- 7: end if
- 8: Calculate λ_n as in (B.5)
- 9: Set $q_{n+1} = (1 \lambda_n)q_n + \lambda_n q_{n+1/2}$
- 10: end for

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