



AN ALGORITHMIC FRAMEWORK FOR OPTIMAL CONTROL OF HYBRID DYNAMICAL SYSTEMS WITH PARABOLIC PDES

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Dedicated to the memory of Thomas I. Seidman (1935–2024)

Abstract. We present a new algorithmic approach for the computational solution of optimal control problems with hybrid nature governed by linear parabolic partial differential equations (PDEs) featuring state-dependent switches. We propose a stepwise reformulation of the initial model by methods from disjunctive programming (DP) and a time transformation method. Under a transversality assumption, we first remove the state-dependent switching rule by introduction of explicit switching variables and vanishing constraints (VCs). Subsequently, we reformulate the obtained optimization task as a mathematical problem with equilibrium constraints (MPEC). Afterwards, the combination of the previous reformulation steps with a regularization of the state equation and Moreau-Yosida type penalization yields a surrogate model with only finite dimensional constraints. Ultimately, this approach allows us to derive necessary first-order optimality conditions to filter candidates for optimality. After detailed discussion of each reformulation step, we introduce the algorithmic framework based on the semismooth Newton method. Finally, we report on promising computational results within the presented framework.

Keywords. Equilibrium constraints; Hybrid systems; Implicit switching; Semismooth Newton; Vanishing constraints.

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1. INTRODUCTION

Countless technical and economical processes can be formulated as optimal control problems. Applications involving implicit switching behavior are, for instance, safety circuits for heating processes where the procedure is interrupted once a critical temperature threshold is obtained [36]. Another example is controlling bacteria growth within a petri dish where the metabolic activity of the bacteria is determined by the overall cell concentration within the dish [37]. Finally, we mention the application to gas networks where the transport through the network is to be optimized, while flap-valves open/close state-dependently to prevent flow reversal for example on compressor in- and outlets [20].

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In the context of optimization, the presence of logical conditions in such problems can be addressed using disjunctive programming (DP). For mixed-integer optimal control problems (MIOCPs), these techniques were already used to obtain regularity results for the optimal value function [18].

For state-dependent switching rules as in the above tasks, a core-difficulty is the implicit description of the involved switches. In the framework of ordinary differential equations (ODEs), it is well-known that DP can be used for explicit reformulations. The implicit switching rule can, e.g., be replaced by explicit switching variables and vanishing constraints (VCs), as proposed by Bock et al. [6]. The authors in [6] then proceed to solve a MIOCP by relaxed partial outer convexification and Sum-Up-Rounding (SUR). A related approach is discussed by Biegler and Baumdrucker in [5], where the combinatorial aspects of the switching rule are formulated as equilibrium constraints (ECs). Both aforementioned approaches are direct methods, i.e., they follow the first discretize then optimize paradigm.

In the ODE framework, the application of the hybrid maximum principle (HMP) in appropriate manner yields a set of necessary optimality conditions for the indirect approach. There exist various formulations of the HMP that each involve different combinations of state and control constraints. For instance, [40] considers non-smooth dynamics and in [41] smooth systems with state constraints have been studied. In [11] another variant of the HMP is obtained by application of a transformation method that reformulates the investigated system in such a way that the application of the basic maximum principle (MP) is again possible; see, e.g., [31]. The transformation presented therein displays many parallels to the one utilized in this paper. Although the HMP is established in the ODE framework, the situation changes drastically, when the dynamics are governed by partial differential equations (PDEs). Li et al. [30] have formulated the MP for elliptic and parabolic equations. Casas has also included state constraints in [7]. However, a generalized statement on the HMP for PDEs is still unavailable. A first step in this direction has been performed for instance in [34], where adjoint based representations for the sensitivity of the objective function with respect to the switching times and the switching sequence have been derived.

In this work, we aim to algorithmically solve systems with implicit switching governed by linear parabolic PDEs. Therefore, we proceed along the path established for ODEs and perform various non-trivial adjustments to make the indirect approach also available to PDEs.

In the following work, we first proceed as in [6, 19] and obtain a MIOCP formulation with vanishing constraints. In contrast to [19], where we solve a relaxed formulation and afterwards apply the VC-adjusted SUR scheme [28] to obtain a feasible discrete control, we apply the time transformation method in the present paper. The time transformation method has been introduced by Lee et al. [29] and further developed by Gerdt in [17] to include optimization over the mode selection. The contribution by Leyendecker et al. allows to even include mode-dependent state constraints [33]. The distinctive feature of the time transformation is the fixation of the discrete modes along the time horizon by the so-called integer control function, which in turn is a step function that attains only values in the range of the discrete control variables. This construction then yields a time grid with fixed values for the discrete control. To optimize the choice of the discrete-valued controls on this grid, a new continuous control variable, the so-called time control, is introduced. This control steers the time spent in a given discrete mode for the transformed system and hence can be interpreted as the propagation velocity through

the discrete grid. A major advantage for the resulting problem formulation is the appearance of only continuous-valued controls. However, the dynamic has to be adjusted towards the new time grid, which is defined by the integer control. The required transformation in the principal part of the dynamics appears inconspicuous and is indeed harmless within the ODE framework, whereas it presents a major challenge for the PDE framework, since it drastically modifies the type of the involved PDEs. This observation requires the introduction of a new solution concept, namely forward solutions, for the PDE framework and results in an additional regularization step in contrast to the ODE framework. In this context, we demonstrate pointwise convergence of the regularized state towards the forward solution as our main contribution.

Another reformulation step is the embedding of the resulting formulation into the EC framework in order to apply penalization approach therein. Both VCs and ECs require cautious treatment since a local minimizer of these programs usually violates standard constraints qualifications (CQs), even in a finite dimensional setting. In this regard, we mention the contributions to mathematical programs with equilibrium constraints (MPECs) by Kanzow et al. in [2, 14, 15, 16] and refer to [42] for the extension to Banach spaces.

A brief theoretical comparison with our approach in [19] yields the following core differences. The application of the time transformation does not admit the same desirable convexification properties with respect to the dynamic as the relaxation approach in [19]. In contrast, the appearance of the additional control term in the principal part of the dynamics even introduces additional non-convexities into the dynamics. However, application of the time transformation yields a formulation with only finitely many VCs to take the implicit switching rule into account. Ultimately, the penalized formulation requires only a finite number of constraints as well. This provides a significant advantage for the derivation of the associated optimality conditions on which the algorithmic framework is founded.

Our penalty approach is based on the results for optimal control problems with semilinear parabolic PDEs and explicit switches by Kunisch et al. [10]. However, the problem formulation discussed in [10] does allow neither the incorporation of the state constraints, which arise from the implicit switching rule, nor equilibrium constraints. But, the techniques presented therein still prove to be helpful once those constraints are removed by penalization. Penalization techniques for PDEs with state constraints have, for instance, been discussed by Hintermüller and Kunisch in [22] and Ito and Kunisch in [26]. Differentiable penalization of equilibrium constraints has been investigated by Huang et al. [24] or Hu and Ralph [25]. Altogether, the combination of the mentioned methods seems promising and enables an indirect approach.

This article is organized as follows. In Section 2, the problem formulation together with an example is introduced. Section 3 discusses in detail the aforementioned reformulation from implicit switching to explicit switching and vanishing constraints, before arriving at a formulation with explicit switching variables and equilibrium constraints. Ultimately, this section is concluded the penalized formulation and the derivation of necessary optimality conditions. In Section 4, we introduce our algorithm based on a semismooth Newton scheme to algorithmically solve the necessary optimality conditions, obtained at the end of Section 3. In Section 5, we report on the performance of the proposed algorithm in a numerical experiment and in Section 6 the core innovations are summarized and future research branches are addressed.

2. PROBLEM FORMULATION

Let $t_f > t_0 \geq 0$ and $\Omega \subset \mathbb{R}^n$ be a bounded domain with C^2 boundary for $n \in \mathbb{N}$

$$\min_{y \in Y, u \in U, v \in V} J(y, u) := \frac{1}{2} \|y - y_d\|_{L^2_{[t_0, t_f]}(H)}^2 + \frac{\gamma u}{2} \|u\|_{L^2_{[t_0, t_f]}(H)}^2 \quad (2.1a)$$

$$\text{s.t. } y_t(t) = Ay(t) + F_{v(t)}u(t) \quad t \in [t_0, t_f], \quad (2.1b)$$

$$y(t_0) = y_0, \quad (2.1c)$$

$$v(t) = C(y(t)) \quad t \in [t_0, t_f], \quad (2.1d)$$

$$C = R \circ S. \quad (2.1e)$$

In the provided setting, $C : H \rightarrow [D] := \{1, \dots, D\}$ denotes the mode function on a Hilbert space H for a fixed number of modes $D \in \mathbb{N}$. We set $Y := C^0_{[t_0, t_f]}(H)$, $U := L^2_{[t_0, t_f]}(H)$, and $V := L^\infty_{[t_0, t_f]}([D])$. Moreover, the symbols $A, (F_d)_{d \in [D]}, R, S$ represent suitable operators, which will be introduced in detail below. We note that the objective function J in (2.1) does not contain any switching cost to prevent an accumulation point of switching times, the so-called Zeno behavior, e.g., [21]. Instead, we postulate Assumption 2.3. Prior to that, we present the assumptions on the problem formulation.

Assumption 2.1.

- (1) Let H, Z be separable Hilbert spaces with continuous and dense embedding $Z \hookrightarrow H$. We consider a Gelfand triple $Z \hookrightarrow H \hookrightarrow Z^*$ with continuous and dense embeddings.
- (2) The operator A is a linear, symmetric, and uniformly elliptic differential operator of second order in divergence form

$$Ay = \sum_{i,j=1}^n \frac{\partial}{\partial x_i} \left(a_{ij}(x) \frac{\partial y}{\partial x_j} \right) + b(x)y$$

for fixed coefficient functions $a_{ij} \in L^\infty(\Omega)$ and $b \in L^\infty(\Omega)$ with $b \geq 0$ such that for a constant $c > 0$ and all $x \in \Omega$ the inequality

$$\sum_{i,j=1}^n a_{ij}(x) \xi_i \xi_j \geq c \|\xi\|^2 \quad (2.2)$$

holds for all $\xi \in \mathbb{R}^n$.

- (3) There exist constants $\varepsilon_\lambda, c_\lambda, C_\lambda > 0$ such that the eigenvalues λ_k of A satisfy $c_\lambda k^{\varepsilon_\lambda} \leq |\lambda_k| \leq C_\lambda k^{\varepsilon_\lambda}$ for all $k \in \mathbb{N}$.
- (4) The operator A generates a C_0 -semigroup $(T(t))_{t \geq 0} \subset \mathcal{L}(H, H)$ such that the spectral determining growth conditions holds

$$\inf_{t > 0} \frac{1}{t} \log(\|T(t)\|_{\mathcal{L}(H, H)}) =: \omega_0 = \sup_{k \in \mathbb{N}} \Re(\lambda_k).$$

- (5) For some $\lambda > \omega_0$ the resolvent $R(\lambda, A) := (\lambda \text{Id} - A)^{-1}$ of the operator A is compact.
- (6) The mapping $F_d : H \rightarrow H, z \mapsto F_d(z)$ is linear and continuous for all modes $d \in [D]$.
- (7) The initial state and desired state fulfill $y_0 \in H$ and $y_d \in U$, respectively. Furthermore, $D_t y_d \in U$ and $D_{tt}^2 y_d \in U$ holds.

Assumption 2.2.

- (1) $S : H \rightarrow \mathbb{R}$ is a linear and continuous function.

(2) $R : \mathbb{R} \rightarrow [D]$ is piecewise constant and the inverse image of each mode $d \in [D]$ is either a closed or an open interval, i.e., there are real numbers $a_d < b_d$ such that

$$R^{-1}(d) = [a_d, b_d] \text{ or } R^{-1}(d) = (a_d, b_d) \quad \forall d \in [D].$$

Here, we apply the convention $a_d := -\infty$ and $b_d := \infty$ if $R^{-1}(d)$ is not bounded from below and if $R^{-1}(d)$ is not bounded from above, respectively. In said cases, the improper values a_d, b_d are always excluded from $R^{-1}(d)$.

We utilize the semigroup $(T(t))_{t \geq 0}$ generated by A to represent the solution to the state equation (2.1b) – (2.1c). For $t \in [t_0, t_f]$ the mild solution $y \in Y$ to (2.1b) – (2.1c) associated with $(u, v) \in U \times V$ is given by

$$y(t) = T(t - t_0)y_0 + \int_{t_0}^t T(t - s)F_{v(s)}u(s) ds. \quad (2.3)$$

Assumption 2.3. Let $y \in Y$ be the mild solution to (2.1b) – (2.1c) generated by some $(u, v) \in U \times V$ and consider $\pi_s \in [t_0, t_f]$ such that

$$S(y(\pi_s)) \in \Sigma_D := \bigcup_{d \in [D]} \{a_d, b_d\}. \quad (2.4)$$

We say that the problem (2.1) satisfies the so-called transversality assumption if the derivatives of $t \mapsto S(y(t))$ from the left and from the right

$$S'_-(y(\pi_s)) := \lim_{t \uparrow \pi_s} \frac{S(y(\pi_s)) - S(y(t))}{\pi_s - t}, \quad S'_+(y(\pi_s)) := \lim_{t \downarrow \pi_s} \frac{S(y(t)) - S(y(\pi_s))}{t - \pi_s},$$

exist at π_s and $S'_+(y(\pi_s)) \cdot S'_-(y(\pi_s)) > 0$ holds for all π_s that fulfill (2.4) and for all (u, v) .

From Assumption 2.3, we conclude that the number of switching times is finite.

Lemma 2.4. [19, Lemma 2.5] *Let Assumptions 2.1, 2.2, and 2.3 hold and denote by $y \in Y$ the mild solution to (2.1b) – (2.1c) generated by $(u, v) \in U \times V$. Then, $C(y(\cdot))$ possesses only a finite number of discontinuities in $[t_0, t_f]$, i.e., $C(y(\cdot))$ is piecewise constant.*

An immediate consequence of Lemma 2.4 is the absence of Zeno-behavior in (2.1) under Assumption 2.3.

Remark 2.5. In this work, Assumption 2.3 is crucial to ensure that the mild solution (2.3) is well-posed in terms of existence, uniqueness, and continuous dependency on parameters [35]. In its absence solutions to hybrid dynamical systems can also be declared in a broader, i.e., in a set-valued sense [13]. This allows to include phenomena like bifurcations or sliding modes. The presented results are then to some extent still applicable but require a more cautious interpretation. For instance, continuous dependency is to be replaced by upper-semicontinuity of the solution set [37]. The solutions to the subsequent reformulations then describes one potential solution branch. This is in particular to be kept in mind for the numerical approach.

In view of Lemma 2.4, we introduce for an admissible triple (y, u, v) to (2.1) the corresponding switching schedule $S = \{(t_0, d_1), \dots, (\pi_j, d_{j+1}), \dots, (\pi_\zeta, d_{\zeta+1})\}$. Here, $\zeta \in \mathbb{N}_0$ describes the number of switches and d_{j+1} , for $j \in [\zeta]$, denotes the evaluation of v after the j -th switch has taken place at time $\pi_j \in [t_0, t_f]$. Hence, we derive from (2.3) the following representation for y

$$y(t) = T(t - t_0)y_0 + \int_{t_0}^t T(t - s) \sum_{j=1}^{\zeta+1} \chi_{(\pi_{j-1}, \pi_j)}(s) F_{d_j} u(s) ds. \quad (2.5)$$

Herein, we set $\pi_0 := t_0$ and $\pi_{\zeta+1} := t_f$. Furthermore, let $\chi_M : \mathbb{R}^n \rightarrow \mathbb{R}$ denote the characteristic function for a Lebesgue measurable set $M \subset \mathbb{R}^n$, i.e., $\chi_M(x) = 1$ if $x \in M$ and $\chi_M(x) = 0$ if $x \notin M$. Under the presented assumptions, we can reformulate (2.1) as

$$\begin{aligned} \min_{y \in Y, u \in U, v \in V} J(y, u) \\ \text{s.t. } y_t(t) = Ay(t) + F_{v(t)}u(t) \end{aligned} \quad t \in [t_0, t_f], \quad (2.6a)$$

$$y(t_0) = y_0, \quad (2.6b)$$

$$0 \leq S(y(t)) - a_{v(t)} \quad t \in [t_0, t_f], \quad (2.6c)$$

$$0 \leq b_{v(t)} - S(y(t)) \quad t \in [t_0, t_f]. \quad (2.6d)$$

Lemma 2.6. [19, Lemma 3.1] *Let Assumptions 2.1, 2.2, and 2.3 hold for (2.1) and (2.6), then the formulations (2.1) and (2.6) are equivalent.*

To illustrate the discussed switching mechanism, we consider the following example, which results after minor modification from [19, Example 5.1].

Example 2.7. Suppose we attempt to solve the tracking task towards a given desired state y_d by solutions of the heat equation, labelled with y , involving the Laplace operator with respect to $x \in \Omega$, denoted by Δy , while also taking into account the required control effort. The control-dependent part of the state equation is formed by the control u , which is restricted to, possibly disjoint, control domains Ω_d for every $d \in [D]$. The active control is determined by the spatial mean value of the state at each time $t \in [t_0, t_f]$, in dependence of a threshold $\sigma \in \mathbb{R}$. More precisely, let $D = 2$, $\Omega_d \subset \Omega \subset \mathbb{R}^n$ for $d \in [D]$ be bounded domains, $Q := \Omega \times (t_0, t_f)$ the space-time cylinder, and $\Sigma := \partial\Omega \times (t_0, t_f)$. For a parameter $r \geq 0$, we consider the optimization problem

$$\begin{aligned} \min_{y \in Y, u \in U, v \in V} J(y, u) &= \frac{1}{2} \|y - y_d\|_{L^2_{[t_0, t_f]}(L^2(\Omega))}^2 + \frac{\gamma_u}{2} \|u\|_{L^2_{[t_0, t_f]}(L^2(\Omega))}^2 \\ \text{s.t. } y_t(x, t) &= (1+r)\Delta y(x, t) + (1+r)u(x, t)\chi_{\Omega_{v(t)}}(x) & (x, t) \in Q, \\ y(x, t) &= 0 & (x, t) \in \Sigma, \\ y(x, t_0) &= y_0(x) & x \in \Omega, \\ v(t) &= \begin{cases} 1 & \text{if } \int_{\Omega} y(x, t) dx < \sigma, \\ 2 & \text{if } \int_{\Omega} y(x, t) dx \geq \sigma, \end{cases} & t \in [t_0, t_f]. \end{aligned}$$

In order to fit this into the setting (2.1), we set $H = L^2(\Omega)$, $Z = H_0^1(\Omega)$, and $Ay = (1+r)\Delta y$ for $D(A) = H_0^1(\Omega) \cap H^2(\Omega)$. Ultimately, we define the mappings

$$\begin{aligned} F_d : L^2(\Omega) &\rightarrow L^2(\Omega), u \mapsto (1+r)u\chi_{\Omega_d}, \\ C : L^2(\Omega) &\rightarrow \{1, 2\}, y \mapsto \begin{cases} 1 & \text{if } \int_{\Omega} y(x) dx < \sigma, \\ 2 & \text{if } \int_{\Omega} y(x) dx \geq \sigma, \end{cases} \\ S : L^2(\Omega) &\rightarrow \mathbb{R}, y \mapsto \int_{\Omega} y(x) dx, \\ R : \mathbb{R} &\rightarrow \{1, 2\}, z \mapsto \begin{cases} 1 & \text{if } z < \sigma, \\ 2 & \text{if } z \geq \sigma. \end{cases} \end{aligned}$$

3. REFORMULATIONS

In this section, we discuss reformulations that allow a tractable approach to solve (2.1). First, we establish a transformation that removes the implicit switching rule from the problem original formulation. Instead, the newly obtained problem features the switching points as explicit control variables and accounts for the switching rule with vanishing state constraints. Hence, the transformed formulation is classified as a mathematical program with vanishing constraints (MPVC). However, MPVCs are well-known as difficult tasks in particular with regard to optimality conditions.

In a second reformulation step, we transform the vanishing constraints into equilibrium constraints by introduction of an additional slack variable. Thereby, we obtain a mathematical program with equilibrium constraints (MPEC). However, the MPEC reformulation still includes mixed control-state constraints connected with the switching rule. Therefore, it again does not allow the immediate formulation of necessary optimality conditions.

Finally, we penalize both the mixed control-state constraints and equilibrium constraints such that the obtained formulation admits the characterization of local minimizers by first-order optimality conditions and eventually allows application of well-established optimization routines, e.g., semismooth Newton method.

3.1. Transformation from implicit to explicit switching via a time transformation method.

In this subsection, we examine the removal of the implicit switching rule from formulation (2.1). Also, the equivalent formulation (2.6) still includes the state-dependent choice of $v(t)$. We utilize the time transformation method [17, 29, 33] to include the switching times as explicit controls. For that purpose, we require to partition the time domain $[t_0, t_f]$. We begin with several assumptions on the involved partition.

Assumption 3.1.

- (1) The time interval $[t_0, t_f]$ is partitioned into \mathcal{M} pairwise disjoint and open intervals $I_i := (t_{(i-1)}, t_i)$, i.e., $[t_0, t_f] = \bigcup_{i \in [\mathcal{M}]} \bar{I}_i$. We refer to an element I_i of this first partition as a *major interval*.
- (2) Each \bar{I}_i is partitioned into $|I_i|$ pairwise disjoint and open intervals $I_i^j := (\tau_{i(j-1)}, \tau_{ij})$, i.e., $\bar{I}_i = \bigcup_{j \in [|I_i|]} I_i^j$. We refer to an element I_i^j of this second partition as a *minor interval*.
- (3) The number of minor intervals $|I_i|$ in Assumption 3.1.2 is the same for each major interval I_i , namely \mathcal{N} .
- (4) The partition is ordered, i.e., $\sup(I_i) = \inf(I_{i+1})$ and $\sup(I_i^j) = \inf(I_i^{j+1})$ holds.
- (5) Each major interval and minor interval possesses the same length. The corresponding lengths of a major and minor interval are denoted by $\Delta_M I$ and $\Delta_m I$, respectively.

To address the elements in the partition by a single index, we set $m(i, j) = (i - 1) \cdot \mathcal{N} + j \in [\mathcal{M} \cdot \mathcal{N}] := [\mathcal{S}]$ for an index pair $(i, j) \in [\mathcal{M}] \times [\mathcal{N}] := \mathcal{P}$. Consequently, we identify

$$\bigcup_{(i,j) \in \mathcal{P}} I_i^j = \bigcup_{m \in [\mathcal{S}]} I_m.$$

Definition 3.2. We call a partition $\bigcup_{(i,j) \in \mathcal{P}} I_i^j$, that fulfills all prerequisites of Assumption 3.1, an *ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length*.

We perform the second partition step to fix the selection of the discrete mode $d \in [D]$ on each minor interval. This is achieved by an integer-valued control function $v_{\mathcal{M}}^{\mathcal{N}}$.

Definition 3.3. Given a number of modes $D \in \mathbb{N}$ and an ordered partition of $[t_0, t_f]$ into minor and major intervals of equal length $\bigcup_{(i,j) \in \mathcal{P}} I_i^j$, we call a function $v_{\mathcal{M}}^{\mathcal{N}} : [t_0, t_f] \rightarrow [D]$, that is constant on each minor interval I_i^j , *integer control function*.

To complete the description of the time transformation method, we introduce the associated time control and time transformation.

Definition 3.4. Let $z \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ be given. We call a function, that fulfills

$$\begin{aligned} z(\tau) &\geq 0 & \tau &\in [t_0, t_f], \\ z|_{I_i^j} &\equiv z_{ij} & (i, j) &\in \mathcal{P}, \\ \Delta_{\text{m}I} &= \int_{I_i} z(s) ds & i &\in [\mathcal{M}], \end{aligned}$$

on a partition $\bigcup_{(i,j) \in \mathcal{P}} I_i^j$, *time control*. Furthermore, we call a minor interval I_i^j *active* if the time control satisfies $z_{ij} > 0$. The minor interval is labelled *inactive*, otherwise.

Definition 3.5. Let $z \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ be a time control. We define the associated *time transformation* $t_z : [t_0, t_f] \rightarrow [t_0, t_f]$ by

$$\tau \mapsto t_z(\tau) := \int_0^{\tau} z(s) ds. \quad (3.1)$$

By (3.1), the time transformation t_z can be explicitly evaluated for an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length. This yields for $\tau \in I_i^j$

$$t_z(\tau) = t_{i-1} + \Delta_{\text{m}I} \sum_{k=1}^{j-1} z_{ik} + (\tau - \tau_{i(j-1)})z_{ij}.$$

The mapping t_z is not injective in the presence of inactive minor intervals and is therefore in general not invertible. However, we can construct a pseudoinverse back-transformation $\tau_z : [t_0, t_f] \rightarrow [t_0, t_f]$,

$$t \mapsto \tau_z(t) := \inf\{s \in [t_0, t_f] \mid t_z(s) = t\}.$$

Now, we focus on the resolution of switches. To resolve all potential switching combinations, we require a suitable number of minor intervals and an appropriate integer control function.

Definition 3.6. We call an integer control function $v_{\mathcal{M}}^{\mathcal{N}} \in V$ associated with a partition $\bigcup_{(i,j) \in \mathcal{P}} I_i^j$ of $[t_0, t_f]$ *consistent* to a discrete control $v \in V$ if for all $i \in [\mathcal{M}]$ and a.e. $t_1, t_2 \in I_i$ with $t_1 < t_2$ there exist $\tau_1, \tau_2 \in I_i$ such that

- (1) $\tau_1 < \tau_2$.
- (2) $v_{\mathcal{M}}^{\mathcal{N}}(\tau_1) = v(t_1), v_{\mathcal{M}}^{\mathcal{N}}(\tau_2) = v(t_2)$.

The integer control $v_{\mathcal{M}}^{\mathcal{N}}$ is called *control consistent* if it is consistent to each discrete control $v \in V$, that admits at most one switch per major interval.

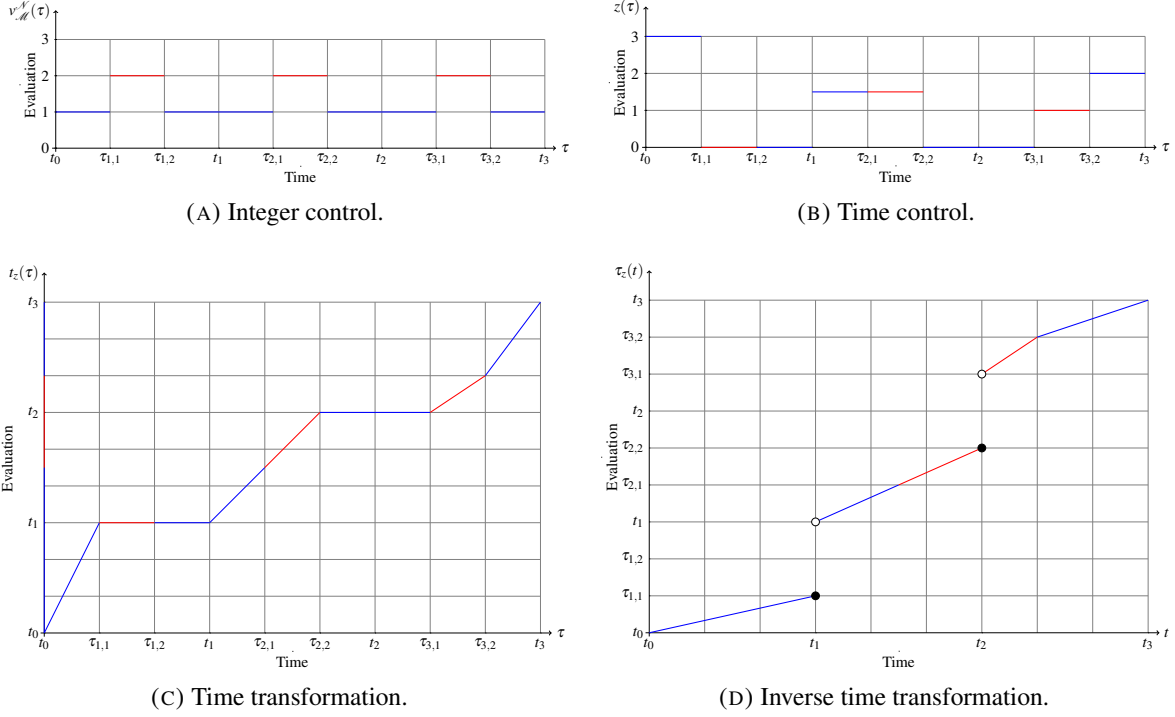


FIGURE 1. Exemplary application of the time transformation method with 3 major and 3 minor intervals.

It can be deduced that a control consistent integer control function requires at least $\mathcal{N} = 2D - 1$ minor intervals. However, this number is also sufficient as demonstrated by the following example.

Example 3.7. Let $D \in \mathbb{N}$ be a fixed number of modes and $\mathcal{N} = 2D - 1$, then we obtain a control consistent integer control function by the following construction

$$v_{\mathcal{M}}^{\mathcal{N}}(\tau) = \begin{cases} j & \text{if } \tau \in I_i^j \text{ for } i \in [\mathcal{M}], 1 \leq j \leq D, \\ 2D - j & \text{if } \tau \in I_i^j \text{ for } i \in [\mathcal{M}], D < j \leq 2D - 1. \end{cases}$$

Now, we can transform (2.6) into a problem with explicit switches and vanishing constraints. In the upcoming formulations, we identify $\tilde{y}_d(\tau) := (y_d \circ t_z)(\tau)$ for $\tau \in [t_0, t_f]$.

We consider the subsequent problem formulation, which incorporates a time control z as an optimization variable, an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal

The white circle icon indicates discontinuities of τ_z at $t \in [t_0, t_f]$, while the black circle icon yields the attained value for $\tau_z(t)$ at the discontinuity.

length $\bigcup_{m \in [\mathcal{I}]} I_m$, and a control consistent integer control function $v_{\mathcal{M}}^{\mathcal{N}}$

$$\begin{aligned} \inf_{y \in Y, u \in U, z \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})} \tilde{J}(y, u, z) &:= \frac{1}{2} \|\sqrt{z} \cdot (y - \tilde{y}_d)\|_U^2 + \frac{\gamma_u}{2} \|\sqrt{z} \cdot u\|_U^2 \\ \text{s.t. } y_{\tau}(\tau) &= z(\tau)Ay(\tau) + z(\tau)F_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)}u(\tau) \quad \tau \in [t_0, t_f], & (3.2a) \\ y(t_0) &= y_0, & (3.2b) \\ z(\tau) &\geq 0 \quad \tau \in [t_0, t_f], & (3.2c) \\ z|_{I_m} &\equiv z_m \quad m \in [\mathcal{I}], & (3.2d) \\ \Delta_M I &= \int_{I_i} z(s) ds \quad i \in [\mathcal{M}], & (3.2e) \\ 0 &\geq z(\tau)(a_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)} - S(y(\tau))) \quad \tau \in [t_0, t_f], & (3.2f) \\ 0 &\geq z(\tau)(S(y(\tau)) - b_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)}) \quad \tau \in [t_0, t_f]. & (3.2g) \end{aligned}$$

Formulation (3.2) contains several novelties and differs noticeably from our previous surrogate model, cf. [19]. One of the distinct innovations is the appearance of the control term z in the principal part of the state equation. Moreover, all appearing variables possess a continuous domain, while the choice of the discrete mode is determined by the fixed $v_{\mathcal{M}}^{\mathcal{N}}$. Also, \tilde{J} is cost-preserving, i.e., let $(\tilde{y}, \tilde{u}, z) := (y \circ t_z, u \circ t_z, z)$ be admissible for (3.2) then $\tilde{J}(\tilde{y}, \tilde{u}, z) = J(y, u)$ holds.

We emphasize the role of the inequalities (3.2f) – (3.2g) for the switching rule. By definition of the switching rule, the state constraints (2.6c) – (2.6d) have to be fulfilled a.e. in $[t_0, t_f]$. However, in formulation (3.2) these constraints have to be satisfied on I_m only if the minor interval is indeed active. This observation is reflected in the constraints (3.2f) – (3.2g). The constraints (3.2f) – (3.2g) are vanishing constraints [2]. A major challenge for MPVCs is the failure of standard constraint qualifications (CQs). This led to the development of MPVC-tailored CQs [1]. From now on, we state our problem formulations with \inf instead of \min since we do not address the existence of global minimizers.

Additionally, formulation (3.2) faces a significant challenge in the state equation (3.2a) – (3.2b), since the constraints (3.2c) – (3.2e) only guarantee that z is a time control. Therefore, they will not prevent z from containing inactive minor intervals. Due to the assumed control consistency of the integer control function $v_{\mathcal{M}}^{\mathcal{N}}$, there will exist several inactive minor intervals I_m for every z . As a result, we can no longer expect the existence of a coercivity constant $c > 0$ for the differential operator $\tilde{A}(\tau) := z(\tau)A$ at all $\tau \in [t_0, t_f]$. Hence, $\tilde{A}(\tau)$ is no longer uniformly elliptic, cf. (2.2). Consequently, the system

$$y_{\tau}(\tau) = z(\tau)Ay(\tau) + z(\tau)F_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)}u(\tau) \quad \tau \in [t_0, t_f], \quad (3.3a)$$

$$y(0) = y_0 \quad (3.3b)$$

requires a solution concept different from mild or weak solutions, cf. [12, 32]. Hence, we study the following set for a fixed integer control $v_{\mathcal{M}}^{\mathcal{N}}$ and time control z

$$V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) := \{y \in Y \mid y|_{I_m} \in W(\tau_{m-1}, \tau_m), \forall m \in [\mathcal{I}] \text{ with } I_m \text{ active}\}.$$

Herein, we abbreviate $W(t_1, t_2) := \{y \in L_{[t_1, t_2]}^2(Z) \mid \dot{y} \in L_{[t_1, t_2]}^2(Z^*)\}$ for $t_1, t_2 \in [t_0, t_f]$. The main idea behind this construction is to continuously, with respect to time and $\|\cdot\|_H$, connect weak solutions on active minor intervals with constant continuations on inactive minor intervals.

Definition 3.8. Let an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{I}]} I_m$, a fixed control consistent integer control function $v_{\mathcal{M}}^{\mathcal{N}} \in V$, and a time control $z \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ be given. Moreover, consider a distributed control $u \in U$ and an initial value $y_0 \in H$. We call a function $y^* \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f)$ *forward solution* of (3.3) for u and y_0 if

- (1) $y^*|_{I_m} \equiv y^*(\tau_m)$ for every inactive I_m .
- (2) $y^*|_{I_m}$ solves

$$\begin{aligned} y_{\tau}(\tau) &= z(\tau)Ay(\tau) + z(\tau)F_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)}u(\tau) & \tau \in I_m, \\ y(\tau_{m-1}) &= y^*(\tau_{m-1}) \end{aligned}$$

for every active I_m .

To state an existence result on forward solutions, we recall a general existence and regularity result for the solution to abstract parabolic equations.

Lemma 3.9. [23, Chapter 1.3.2.4, Theorem 1.35] *Let $y_0 \in H$, $u \in L_{[t_0, t_f]}^2(Z^*)$, and $v \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ be given. Furthermore, there exists $c \in \mathbb{R}$ such that $0 < c < v(t)$ f.a.e. $t \in [t_0, t_f]$. Then, there exists a unique solution $y \in W(t_0, t_f)$ to*

$$\begin{aligned} y_t(t) &= v(t)Ay(t) + u(t) & t \in [t_0, t_f], \\ y(t_0) &= y_0, \end{aligned}$$

which satisfies for $C > 0$ the estimate

$$\|y\|_{W(t_0, t_f)} = \|y\|_{L_{[t_0, t_f]}^2(Z)} + \|\dot{y}\|_{L_{[t_0, t_f]}^2(Z^*)} \leq C(\|u\|_{L_{[t_0, t_f]}^2(Z^*)} + \|y_0\|_H). \quad (3.4)$$

Here, we briefly address the regularity of the state in formulations (2.1) and (2.6).

Remark 3.10. According to Assumption 2.1.6, the evaluation $F_{v(t)}u(t)$ is located in H f.a.e. $t \in [t_0, t_f]$. Furthermore, the set of linear operators $(F_d)_{d \in [D]}$ is finite and therefore uniformly bounded in $\mathcal{L}(H, H)$. Hence, the right-side is located in U and the regularity estimate (3.4) yields $y \in W(t_0, t_f)$. This means that under the stated prerequisites the state equation (2.1b) – (2.1c) possesses a unique mild and weak solution. But, they coincide according to Ball [4]. Hence, we conclude that the states in (2.1) and (2.6) admit the improved regularity $y \in W(t_0, t_f)$.

By induction over the minor intervals, we demonstrate the existence of the forward solution.

Lemma 3.11. *Let an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{I}]} I_m$, a fixed control consistent integer control function $v_{\mathcal{M}}^{\mathcal{N}} \in V$, and a time control $z \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ be given. Moreover, consider a distributed control $u \in U$ and an initial value $y_0 \in H$. Then, there exists a unique forward solution $y^* \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f)$ to (3.3).*

Before we are able to establish the link between formulations (2.6) and (3.2), we require an auxiliary statement regarding a change of variable in the time domain.

Lemma 3.12. *Let $I = (\tau_1, \tau_2), J = (t_1, t_2) \subset \mathbb{R}$ be open intervals and $\varphi : I \rightarrow J$, $\tau \mapsto \varphi(\tau)$ be a C^1 -diffeomorphism such that $\|\varphi'\|_{L_{[\tau_1, \tau_2]}^{\infty}(\mathbb{R})}$ and $\|(\varphi^{-1})'\|_{L_{[t_1, t_2]}^{\infty}(\mathbb{R})}$ are finite. Then, $y \in W(t_1, t_2)$*

is a weak solution to

$$\begin{aligned} y_t(t) &= Ay(t) + u(t) & t \in J, \\ y(t_1) &= y_0, \end{aligned}$$

for $u \in L^2_{[t_1, t_2]}(Z^*)$ and $y_0 \in H$ if and only if $\tilde{y} := y \circ \varphi \in W(\tau_1, \tau_2)$ is the weak solution to

$$\begin{aligned} y_\tau(\tau) &= \varphi'(\tau)Ay(t) + \varphi'(\tau)u(\tau) & \tau \in I, \\ y(\tau_1) &= y_0, \end{aligned}$$

for $\tilde{u} := u \circ \varphi$ and y_0 .

With the previous lemma at hand, we can construct an admissible point for (3.2) from an admissible point to (2.6).

Lemma 3.13. *Let $(y, u, v) \in W(t_0, t_f) \times U \times V$ be admissible for (2.6) with switching schedule $S = \{(t_0, d_1), \dots, (\pi_j, d_{j+1}), \dots, (\pi_\zeta, d_{\zeta+1})\}$ and take $v_{\mathcal{M}}^{\mathcal{N}} \in V$ as a control consistent integer function associated with an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{S}]} I_m$. Moreover, assume that there is at most one discontinuity of v in each major interval I_i by choosing $\Delta_M I < \min_{j \in [\zeta]} \pi_j - \pi_{j-1}$. Then, there exists a time control z such that the triple $(\tilde{y}, \tilde{u}, z) \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) \times U \times L^\infty_{[t_0, t_f]}(\mathbb{R})$ is admissible for (3.2). Here, the state $\tilde{y} := y \circ t_z$ solves the state equation (3.2a) and (3.2b) for the control $\tilde{u} := u \circ t_z$ and initial condition y_0 in the sense of a forward solution.*

Proof. The time control z is constructed as in [33, Theorem 26]. Afterwards, the forward solution properties of \tilde{y} for \tilde{u} and y_0 are concluded with Lemma 3.12. \square

In the previous lemma, we have established the construction of admissible points to (3.2) from admissible points to (2.6). Now, we consider the reversed statement.

Lemma 3.14. *Let $v_{\mathcal{M}}^{\mathcal{N}} \in V$ be a control consistent integer function, associated with an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{S}]} I_m$, and take $(\tilde{y}, \tilde{u}, z) \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) \times U \times L^\infty_{[t_0, t_f]}(\mathbb{R})$ as an admissible triple for (3.2). Then, $(y_*, u_*, v_*) \in W(t_0, t_f) \times U \times V$ defined by $y_* := \tilde{y} \circ \tau_z$, $u_* := \tilde{u} \circ \tau_z$, and $v_* := v_{\mathcal{M}}^{\mathcal{N}} \circ \tau_z$ is admissible for (2.6).*

Proof. By Definition 3.8, the restriction of the forward solution \tilde{y} to $I_a = (\tau_{a-1}, \tau_a) \subset [t_0, t_f]$ satisfies $\tilde{y}|_{I_a} \in W(\tau_{a-1}, \tau_a)$ for every index $a \in \mathcal{A} := \{m \in [\mathcal{S}] \mid I_m \text{ is active}\} = \bigcup_{k=1}^{|\mathcal{S}|} a_k$. Moreover, $\tilde{y}|_{I_a}$ solves for $\tilde{u}|_{I_a} \in L^2_{[\tau_{a-1}, \tau_a]}(H)$ the system

$$y_\tau(\tau) = z_a Ay(\tau) + z_a F_{d_a} u(\tau) \quad \tau \in I_a, \quad (3.5a)$$

$$y(\tau_{a-1}) = \tilde{y}(\tau_{a-1}). \quad (3.5b)$$

For all $a \in \mathcal{A}$ the mapping $t_z|_{I_a} : I_a \rightarrow t_z(I_a)$ is a C^1 -diffeomorphism with bounded Jacobians. The corresponding inverse is given by $\tau_z|_{t_z(I_a)}$ with $\tau'_z(t) = \frac{1}{z_a}$ for all $t \in t_z(I_a)$. Again, by Lemma 3.12, $y_*|_{t_z(I_a)} \in W(t_z(\tau_{a-1}), t_z(\tau_a))$ solves for $u_*|_{t_z(I_a)} \in L^2_{[t_z(\tau_{a-1}), t_z(\tau_a)]}(H)$ the system

$$y_t(t) = Ay(t) + F_{d_a} u(t) \quad t \in t_z(I_a), \quad (3.6a)$$

$$y(t_z(\tau_{a-1})) = \tilde{y}(\tau_{a-1}). \quad (3.6b)$$

Hence, $y_*(t)$ can be for $t \in t_z(I_a)$ expressed as

$$y_*(t) = T(t - t_z(\tau_{a-1}))\tilde{y}(\tau_{a-1}) + \int_{t_z(\tau_{a-1})}^t T(t-s)F_{d_a}u_*(s) ds. \quad (3.7)$$

It holds $\bigcup_{k=1}^{|\mathcal{A}|} \overline{t_z(I_{a_k})} = [t_0, t_f]$ because z is a time control, cf. (3.2c) – (3.2e). Next, we demonstrate that for every $a \in \mathcal{A}$ the restriction of the mild solution, to (2.6a) – (2.6b) for (u_*, v_*) , to $\overline{t_z(I_a)}$ is represented by (3.7). We perform a proof by induction over the indices in $\mathcal{A}_0 := \mathcal{A}$.

For $a_1 := \min(\mathcal{A}_0)$, we conclude $\tilde{y}(\tau_{a_1-1}) = \tilde{y}(\tau_0) = y_0$ because \tilde{y} is a forward solution and hence possesses a constant continuation along inactive minor intervals. The evaluation of the corresponding time transformation yields $t_z(\tau_{a_1-1}) = 0$. Furthermore, y_* satisfies the constraints (2.6c) – (2.6d) on $t_z(I_{a_1})$ with d_{a_1} since (3.2f) – (3.2g) hold for \tilde{y} on I_{a_1} with d_{a_1} . Hence, the expression (3.7) indeed represents the mild solution, to (2.6a) – (2.6b) for (u_*, v_*) , on $\overline{t_z(I_{a_1})}$.

Let the statement be true for a fixed $l \in \mathbb{N}$. We consider $a_l := \min \mathcal{A}_{l-1}$ and $\mathcal{A}_l := \mathcal{A}_{l-1} \setminus \{a_l\}$.

W.l.o.g. we assume $\mathcal{A}_l \neq \emptyset$. By the induction hypothesis, the restriction of y_* to $\overline{t_z(I_{a_l})}$ matches with the mild solution to (2.6a) – (2.6b), generated by (u_*, v_*) , on $\overline{t_z(I_{a_l})}$. Hence, in particular $\tilde{y}(\tau_{a_l}) = y_*(t_z(\tau_{a_l}))$ holds. The definitions of a_{l+1} and the forward solution \tilde{y} yield $\tilde{y}(\tau_{a_l}) = \tilde{y}(\tau_{a_{l+1}-1})$. Therefore, the initial condition (3.6b) for y_* on $\overline{t_z(I_{a_{l+1}})}$ is $y_*(t_z(\tau_{a_{l+1}-1})) = y_*(t_z(\tau_{a_l}))$, i.e., the terminal value of y_* from the previous interval $t_z(I_{a_l})$ is also the initial value for the current interval, $t_z(I_{a_{l+1}})$. By (3.2f) – (3.2g), the state y_* satisfies the constraints (2.6c) – (2.6d) on $t_z(I_{a_{l+1}})$ with $d_{a_{l+1}}$. Again by (3.7), the restriction of y_* to $\overline{t_z(I_{a_{l+1}})}$ matches with the mild solution, to (2.6a) – (2.6b) for (u_*, v_*) , on $\overline{t_z(I_{a_{l+1}})}$.

The previous considerations also demonstrate that $y_* \in Y$. Therefore, y_* can on $t_z(I_a)$ be expressed by (3.7) and admits for $t \in [t_0, t_f]$ the global representation, cf. (2.5)

$$y_*(t) = T(t - t_0)y_0 + \int_{t_0}^t T(t-s) \sum_{k=1}^{|\mathcal{A}|} \chi_{(t_z(\tau_{a_{k-1}}), t_z(\tau_{a_k}))}(s) F_{d_{a_k}} u_*(s) ds.$$

Hence, y_* is the unique mild solution to (2.6a) – (2.6b) for (u_*, v_*) , while also satisfying the constraints (2.6c) – (2.6d) f.a.e. $t \in [t_0, t_f]$. This means (y_*, u_*, v_*) is admissible for (2.6). Again by Remark 3.10, we deduce the improved regularity $y_* \in W(t_0, t_f)$ since $u_* \in U$. \square

As a result from the previous paragraphs, we have transformed the problem formulation with implicit switches (2.6) into a setting with explicit switches and vanishing constraints (3.2). However, the associated MPVC formulation is closely related to an MPEC which have been studied intensively in the recent decades [2, 14, 15, 16]. In particular, results on penalty methods have been discovered [24, 25]. Hence, we embed our optimal control problem into the MPEC framework.

A direct link between local minima of MPVCs and MPECs can be established, cf. [2, Lemma 6.1]. We apply the transformation presented therein to (3.2). This results in the subsequent formulation

$$\begin{aligned}
& \inf_{\substack{y \in Y, \\ z \in L_{[t_0, t_f]}^\infty(\mathbb{R}), \\ u \in U, \\ s \in \mathbb{R}^{2\mathcal{S}}} } \tilde{J}(y, u, z) \\
\text{s.t. } & y_\tau(\tau) = z(\tau)Ay(\tau) + z(\tau)F_{v_{\mathcal{M}}^{\mathcal{N}}}(\tau)u(\tau) & \tau \in [t_0, t_f], & (3.8a) \\
& y(t_0) = y_0, & & (3.8b) \\
& z(\tau) \geq 0 & \tau \in [t_0, t_f], & (3.8c) \\
& z|_{I_m} \equiv z_m & m \in [\mathcal{S}], & (3.8d) \\
& \Delta_M I = \int_{I_i} z(s) ds & i \in [\mathcal{M}], & (3.8e) \\
& s_{a,m} \geq a_{v_{\mathcal{M}}^{\mathcal{N}}}(\tau) - S(y(\tau)) & \tau \in I_m, m \in [\mathcal{S}], & (3.8f) \\
& s_{b,m} \geq S(y(\tau)) - b_{v_{\mathcal{M}}^{\mathcal{N}}}(\tau) & \tau \in I_m, m \in [\mathcal{S}], & (3.8g) \\
& s_{k,m} \geq 0 & (k, m) \in \mathcal{S} \times [\mathcal{S}], & (3.8h) \\
& s_{k,m} \cdot z_m = 0 & (k, m) \in \mathcal{S} \times [\mathcal{S}]. & (3.8i)
\end{aligned}$$

Here, we set $\mathcal{S} := \{a, b\}$, $(s_a, s_b)^\top = s^\top \in \mathbb{R}^{2\mathcal{S}}$, and identify $s_{k,m} = (s_k)_m$ for $(k, m) \in \mathcal{S} \times [\mathcal{S}]$. A minor adjustment in the proof of [19, Lemma 3.12] yields following statement regarding admissibility.

Lemma 3.15. *Let $v_{\mathcal{M}}^{\mathcal{N}} \in V$ be a control consistent integer function, associated with an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{S}]} I_m$. The subsequent*

connections between admissible points for (3.2) and (3.8) hold:

- i) *Let $(y, u, z) \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) \times U \times L_{[t_0, t_f]}^\infty(\mathbb{R})$ be admissible for (3.2) then the element $(y, u, z, s) \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) \times U \times L_{[t_0, t_f]}^\infty(\mathbb{R}) \times \mathbb{R}^{2\mathcal{S}}$ is admissible (3.8), where we initialize the entries of s for $m \in [\mathcal{S}]$ as*

$$\begin{aligned}
s_{a,m} &= \begin{cases} 0 & \text{if } z_m > 0, \\ \max\{0, a_{d_m} - \min_{t \in I_m} S(y(t))\} & \text{else,} \end{cases} \\
s_{b,m} &= \begin{cases} 0 & \text{if } z_m > 0, \\ \max\{0, \max_{t \in I_m} S(y(t)) - b_{d_m}\} & \text{else.} \end{cases}
\end{aligned}$$

- ii) *If $(y, u, z, s) \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) \times U \times L_{[t_0, t_f]}^\infty(\mathbb{R}) \times \mathbb{R}^{2\mathcal{S}}$ is admissible to (3.8), then $(y, u, z) \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f) \times U \times L_{[t_0, t_f]}^\infty(\mathbb{R})$ is admissible for (3.2).*

To obtain a norm-minimal choice of s , we add the relaxation term $\frac{\gamma_s}{2} \|s\|_{\mathbb{R}^{2\mathcal{S}}}^2$ with a parameter $\gamma_s > 0$ to the cost function \tilde{J} .

3.2. A differentiable penalty approach. In this subsection, we apply a differentiable penalty approach because the formulation (3.8) still possesses theoretical drawbacks, which prohibit the formulation of suitable necessary optimality conditions. The most crucial challenge concerns the state equation (3.3), which can only be solved as a forward solution, cf. Subsection 3.1. As a remedy, we propose an approximation of forward solutions by regularized states, which

ultimately enables the formulation of necessary optimality conditions. For a fixed regularization parameter $\varepsilon > 0$, we consider the solution $y_\varepsilon \in W(t_0, t_f)$ to

$$y_\tau(\tau) = (z(\tau) + \varepsilon)Ay(\tau) + (z(\tau) + \varepsilon)F_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)}u(\tau) \quad \tau \in [t_0, t_f], \quad (3.9a)$$

$$y(t_0) = y_0. \quad (3.9b)$$

Thereinafter, we will substitute the state equation in (3.8) by the regularization (3.9). The approximation properties of the weak solution to (3.9) towards the corresponding forward solution of (3.3) are subject of the following two lemmata. We begin with active minor intervals.

Lemma 3.16. *Let an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length*

$\bigcup_{m \in [\mathcal{I}]} I_m$, *a fixed control consistent integer control function $v_{\mathcal{M}}^{\mathcal{N}} \in V$, and a time control $z \in L^\infty_{[t_0, t_f]}(\mathbb{R})$ be given. Furthermore, denote by $y_\varepsilon \in W(t_0, t_f)$ and $y_f \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f)$ the solution to*

(3.9) for a regularization parameter $\varepsilon > 0$ and the forward solution to (3.3), respectively. If $\lim_{\varepsilon \downarrow 0} \|y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1})\|_H = 0$ is satisfied for an active minor interval $I_m = (\tau_{m-1}, \tau_m)$, then

$$\lim_{\varepsilon \downarrow 0} \|y_\varepsilon - y_f\|_{W(\tau_{m-1}, \tau_m)} = 0.$$

Proof. According to the construction of y_ε and y_f , their difference $\delta y_{\varepsilon, f}^m := (y_\varepsilon - y_f)|_{I_m} \in W(\tau_{m-1}, \tau_m)$ satisfies for all $\varepsilon > 0$ the system

$$\begin{aligned} y_\tau(\tau) &= z_m Ay(\tau) + \varepsilon Ay_\varepsilon(\tau) + \varepsilon F_{d_m} u(\tau) & \tau \in I_m, \\ y(\tau_{m-1}) &= y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1}). \end{aligned}$$

From the regularity estimate (3.4), we obtain

$$\begin{aligned} \|\delta y_{\varepsilon, f}^m\|_{W(\tau_{m-1}, \tau_m)} &\leq C(\varepsilon \|Ay_\varepsilon\|_{L^2_{[\tau_{m-1}, \tau_m]}(Z^*)} + \varepsilon \|F_{d_m}\|_{\mathcal{L}(H, H)} \|u\|_{L^2_{[\tau_{m-1}, \tau_m]}(H)} \\ &\quad + \|y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1})\|_H). \end{aligned} \quad (3.10)$$

We conclude that $\|Ay_\varepsilon\|_{L^2_{[\tau_{m-1}, \tau_m]}(Z^*)}$ is uniformly bounded because the operator $A \in \mathcal{L}(Z, Z^*)$ and $\|y_\varepsilon\|_{L^2_{[\tau_{m-1}, \tau_m]}(Z)} < C$ holds for all sufficiently small $\varepsilon > 0$ by repeated application of (3.4). The claim follows by taking the limit $\varepsilon \downarrow 0$ in (3.10). \square

Next, we investigate the approximation properties on inactive minor intervals.

Lemma 3.17. *Let an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length*

$\bigcup_{m \in [\mathcal{I}]} I_m$, *a fixed control consistent integer control function $v_{\mathcal{M}}^{\mathcal{N}} \in V$, and a time control $z \in L^\infty_{[t_0, t_f]}(\mathbb{R})$ be given. Furthermore, denote by $y_\varepsilon \in W(t_0, t_f)$ and $y_f \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f)$ the solution*

to (3.9) for a regularization parameter $\varepsilon > 0$ and the forward solution to (3.3), respectively. If $\lim_{\varepsilon \downarrow 0} \|y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1})\|_H = 0$ is satisfied for an inactive minor interval $I_m = (\tau_{m-1}, \tau_m)$, then

$$\lim_{\varepsilon \downarrow 0} \|y_\varepsilon(\tau) - y_f(\tau)\|_H = 0$$

holds for all $\tau \in \overline{I_m}$.

Proof. We study the regularized solution on inactive minor intervals. The investigated state $y_\varepsilon|_{I_m} \in W(\tau_{m-1}, \tau_m)$ satisfies the system

$$y_\tau(\tau) = \varepsilon A y(\tau) + \varepsilon F_{d_m} u(\tau) \quad \tau \in I_m, \quad (3.11a)$$

$$y(\tau_{m-1}) = y_\varepsilon(\tau_{m-1}), \quad (3.11b)$$

whereas $y_f(\tau) = y_f(\tau_{m-1})$ holds for all $\tau \in \overline{I_m}$ because y_f is a forward solution. We utilize Assumptions 2.1.2 – 2.1.5 to conclude that the C_0 -semigroup $(T(t))_{t \geq 0}$ generated by A is compact and self-adjoint, cf. [3, Corollary 4.4.2]. Hence, A is diagonalizable with an orthonormal basis $(\varphi_k)_{k \in \mathbb{N}}$ of eigenvectors in H , cf. [3, Theorem 4.4.1]. The corresponding family of real eigenvalues $(\lambda_k)_{k \in \mathbb{N}}$ satisfies $\lim_{k \rightarrow \infty} \lambda_k = -\infty$ and $\omega_0 = \sup_{k \in \mathbb{N}} \lambda_k < 0$ according to Assumptions 2.1.3 and 2.1.4. W.l.o.g. we assume $\lambda_k \geq \lambda_{k+1}$. Therefore, we obtain for all $y \in H$ the representation

$$T(\tau)y = \sum_{k=1}^{\infty} \exp(\lambda_k \tau) \langle y, \varphi_k \rangle_H \varphi_k.$$

Similarly, we conclude that for each $\varepsilon > 0$ the C_0 -semigroup $(T_\varepsilon(\tau))_{\tau \geq 0}$ generated by the operator εA can be represented as

$$T_\varepsilon(\tau)y = \sum_{k=1}^{\infty} \exp(\varepsilon \lambda_k \tau) \langle y, \varphi_k \rangle_H \varphi_k. \quad (3.12)$$

The C_0 -semigroup $(T_\varepsilon(\tau))_{\tau \geq 0}$ is for every $\varepsilon > 0$ a semigroup of contractions as we conclude for all $\tau \geq 0$ and $\varepsilon > 0$ the following estimate by Parseval's identity

$$\|T_\varepsilon(\tau)y\|_H^2 = \sum_{k=1}^{\infty} (\exp(\varepsilon \lambda_k \tau) \langle y, \varphi_k \rangle_H)^2 \leq \sum_{k=1}^{\infty} \langle y, \varphi_k \rangle_H^2 = \|y\|_H^2. \quad (3.13)$$

Furthermore, we can express the mild solution to (3.11) for $\tau \in [\tau_{m-1}, \tau_m]$ as

$$y_\varepsilon(\tau) = T_\varepsilon(\tau - \tau_{m-1})y_\varepsilon(\tau_{m-1}) + \varepsilon \int_{\tau_{m-1}}^{\tau} T_\varepsilon(\tau - s)F_{d_m}u(s) ds. \quad (3.14)$$

We derive the following estimate from the contraction property of $(T_\varepsilon(\tau))_{\tau \geq 0}$

$$\begin{aligned} & \|T_\varepsilon(\tau - \tau_{m-1})y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1})\|_H \\ & \leq \|T_\varepsilon(\tau - \tau_{m-1})(y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1}))\|_H + \|T_\varepsilon(\tau - \tau_{m-1})y_f(\tau_{m-1}) - y_f(\tau_{m-1})\|_H \\ & \leq \|y_\varepsilon(\tau_{m-1}) - y_f(\tau_{m-1})\|_H + \|T_\varepsilon(\tau - \tau_{m-1})y_f(\tau_{m-1}) - y_f(\tau_{m-1})\|_H. \end{aligned} \quad (3.15)$$

Eventually, we conclude $\lim_{\varepsilon \downarrow 0} \|T_\varepsilon(\tau - \tau_{m-1})y_f(\tau_{m-1}) - y_f(\tau_{m-1})\|_H = 0$ since $(T_\varepsilon(\tau))_{\tau \geq 0}$ is a C_0 -semigroup and (3.12) is symmetric with respect to τ and ε . By Hölder's inequality and (3.13), we obtain that the integral expression in (3.14) is uniformly bounded for $\varepsilon > 0$

$$\begin{aligned} \left\| \int_{\tau_{m-1}}^{\tau} T_\varepsilon(\tau - s)F_{d_m}u(s) ds \right\|_H & \leq C \int_{\tau_{m-1}}^{\tau} \|T_\varepsilon(\tau - s)F_{d_m}u(s)\|_H^2 ds \\ & \leq C \int_{\tau_{m-1}}^{\tau} \|F_{d_m}u(s)\|_H^2 ds \\ & \leq C \|F_{d_m}\|_{\mathcal{L}(H,H)}^2 \|u\|_U^2. \end{aligned} \quad (3.16)$$

The claim follows by combining (3.15) and (3.16) and taking $\varepsilon \downarrow 0$ in (3.14). \square

After establishing pointwise convergence on both inactive and active minor intervals, we can prove the complete approximation statement by induction.

Theorem 3.18. *Let an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{I}]} I_m$, a fixed control consistent integer control function $v_{\mathcal{M}}^{\mathcal{N}} \in V$, and a time control $z \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ be given. Furthermore, denote by $y_{\varepsilon} \in W(t_0, t_f)$ and $y_f \in V_{v_{\mathcal{M}}^{\mathcal{N}}, z}(t_0, t_f)$ the solution to (3.9) for a regularization parameter $\varepsilon > 0$ and the forward solution to (3.3), respectively. Then,*

$$\lim_{\varepsilon \downarrow 0} \|y_{\varepsilon}(\tau) - y_f(\tau)\|_H = 0$$

holds for all $\tau \in [t_0, t_f]$.

To preserve non-negativity of the objective function, we replace z by $z + \varepsilon$ in \tilde{J} . To emphasize the underlying finite dimensionality, we write $\bar{\alpha} \in L_{[t_0, t_f]}^{\infty}(\mathbb{R})$ for the piecewise constant function, that is uniquely determined by a vector $\alpha \in \mathbb{R}^{\mathcal{I}}$ and the property $\bar{\alpha}|_{I_m} \equiv \alpha_m$, on an ordered partition of $[t_0, t_f]$ into major and minor intervals of equal length $\bigcup_{m \in [\mathcal{I}]} I_m$. Finally, we set $\bar{y}_d(\tau) := (y_d \circ t_{\bar{\alpha}})(\tau)$. We consider for $\varepsilon > 0$ the problem

$$\begin{aligned} \inf_{\substack{y \in W(t_0, t_f), \quad u \in U, \\ \alpha \in \mathbb{R}^{\mathcal{I}}, \quad s \in \mathbb{R}^{2\mathcal{I}}}} J_{\varepsilon}(y, u, \alpha, s) &:= \frac{1}{2} \left\| \sqrt{\bar{\alpha} + \varepsilon} \cdot (y - \bar{y}_d) \right\|_U^2 \\ &+ \frac{\gamma_u}{2} \left\| \sqrt{\bar{\alpha} + \varepsilon} \cdot u \right\|_U^2 + \frac{\gamma_s}{2} \|s\|_{\mathbb{R}^{2\mathcal{I}}}^2 \\ \text{s.t. } y_{\tau}(\tau) &= (\bar{\alpha}(\tau) + \varepsilon)Ay(\tau) + (\bar{\alpha}(\tau) + \varepsilon)F_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)}u(\tau) \quad \tau \in [t_0, t_f], & (3.17a) \\ y(t_0) &= y_0, & (3.17b) \\ \bar{\alpha}(\tau) &\geq 0 \quad \tau \in [t_0, t_f], & (3.17c) \\ \bar{\alpha}|_{I_m} &\equiv \alpha_m \quad m \in [\mathcal{I}], & (3.17d) \\ \Delta_M I &= \int_{I_i} \bar{\alpha}(s) ds \quad i \in [\mathcal{M}], & (3.17e) \\ s_{a,m} &\geq a_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)} - S(y(\tau)) \quad \tau \in I_m, m \in [\mathcal{I}], & (3.17f) \\ s_{b,m} &\geq S(y(\tau)) - b_{v_{\mathcal{M}}^{\mathcal{N}}(\tau)} \quad \tau \in I_m, m \in [\mathcal{I}], & (3.17g) \\ s_{k,m} &\geq 0 \quad (k, m) \in \mathcal{I} \times [\mathcal{I}], & (3.17h) \\ s_{k,m} \cdot \alpha_m &= 0 \quad (k, m) \in \mathcal{I} \times [\mathcal{I}]. & (3.17i) \end{aligned}$$

The presented ε -regularization enables application of standard parabolic theory towards the state equation. However, formulation (3.17) still includes the mixed control-state constraints (3.17f) and (3.17g) together with the equilibrium constraints (3.17c), (3.17h), and (3.17i). Hence, we proceed with a penalty strategy.

We briefly motivate our penalty approach. In [10] optimality conditions for semilinear parabolic equations with explicit switches are discussed. Therein, the authors apply a transformation method with similar properties compared to our time transformation. However, they do not cover mode-dependent state constraints. Traditionally, state constraints require cautious treatment as their associated Lagrange multipliers are expected to possess low regularity. In this context, the technique of Moreau-Yosida penalization is well-established [22, 26]. Also, convergence results for differentiable penalty functions are available for finite dimensional MPECs [24, 25]. Therefore, a combined penalty approach for the present mixed control-state and equilibrium constraints also seems promising.

For the mixed control-state constraints we employ the penalty function $J_{\text{MY}} : U \times \mathbb{R}^{2 \cdot \mathcal{I}} \rightarrow \mathbb{R}$,

$$(y, s) \mapsto \frac{1}{2} \sum_{m=1}^{\mathcal{I}} \int_{I_m} \left(a_{v_{\mathcal{M}}}(\tau) - S(y(\tau)) - s_{a,m} \right)_+^2 d\tau + \int_{I_m} \left(S(y(\tau)) - b_{v_{\mathcal{M}}}(\tau) - s_{b,m} \right)_+^2 d\tau$$

for a penalty parameter $\gamma_{\text{MY}} > 0$. Therein, we set $g(\tau)_+ := \max\{0, g(\tau)\}$ for $\tau \in [t_0, t_f]$. Additionally, we abbreviate

$$h_-(y, s)(\tau) := \left(a_{v_{\mathcal{M}}}(\tau) - y(\tau) - s \right)_+, \quad h_+(y, s)(\tau) := \left(y(\tau) - b_{v_{\mathcal{M}}}(\tau) - s \right)_+$$

for $s \in \mathbb{R}, y \in L^2_{[t_0, t_f]}(\mathbb{R})$. For the penalization of the ECs we utilize a nonlinear complementarity (NCP) function. Each NCP function $\varphi : \mathbb{R}^2 \rightarrow \mathbb{R}$ possesses the property

$$\varphi(\alpha, s) = 0 \iff \alpha \geq 0, s \geq 0, \alpha \cdot s = 0.$$

Hence, the roots of φ are exactly the points that satisfy the EC. Despite being well-studied cf. [39], NCP functions often lack the desired smoothness properties for the derivation of first-order conditions. For the construction of our penalty method, we employ the Fischer-Burmeister function

$$\varphi_{\text{FB}} : \mathbb{R}^2 \rightarrow \mathbb{R}, (\alpha, s) \mapsto \sqrt{\alpha^2 + s^2} - \alpha - s.$$

This specific NCP function exhibits the additional property that φ_{FB}^2 is differentiable and its derivative $D\varphi_{\text{FB}}^2$ is semismooth [8]. Therefore, φ_{FB}^2 possesses exactly the desired smoothness properties for the application of a semismooth Newton method. We penalize the ECs for a penalty parameter $\gamma_{\text{EC}} > 0$ by

$$J_{\text{EC}} : \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{2 \cdot \mathcal{I}} \rightarrow \mathbb{R}, (\alpha, s) \mapsto \frac{1}{2} \sum_{k \in \mathcal{I}} \sum_{m=1}^{\mathcal{I}} \varphi_{\text{FB}}^2(\alpha_m, s_{k,m}).$$

Hence, the penalized version of (3.17) is given by

$$\inf_{\substack{y \in W(t_0, t_f), u \in U, \\ \alpha \in \mathbb{R}^{\mathcal{I}}, s \in \mathbb{R}^{2 \cdot \mathcal{I}}}} J_p(y, u, \alpha, s) := \frac{1}{2} \left\| \sqrt{\bar{\alpha} + \varepsilon} \cdot (y - \bar{y}_d) \right\|_U^2 + \frac{\gamma_u}{2} \left\| \sqrt{\bar{\alpha} + \varepsilon} \cdot u \right\|_U^2$$

$$+ \frac{\gamma_s}{2} \|s\|_{\mathbb{R}^{2 \cdot \mathcal{I}}}^2 + \gamma_{\text{EC}} J_{\text{EC}}(\alpha, s) + \gamma_{\text{MY}} J_{\text{MY}}(y, s)$$

$$\text{s.t. } y_\tau(\tau) = (\bar{\alpha}(\tau) + \varepsilon) A y(\tau) + (\bar{\alpha}(\tau) + \varepsilon) F_{v_{\mathcal{M}}}(\tau) u(\tau) \quad \tau \in [t_0, t_f], \quad (3.18a)$$

$$y(t_0) = y_0, \quad (3.18b)$$

$$\Delta_{\text{M}} I = \sum_{j=1}^{\mathcal{N}} \alpha_{(i-1)\mathcal{N}+j} \quad i \in [\mathcal{M}], \quad (3.18c)$$

$$\alpha_m \geq 0 \quad m \in [\mathcal{I}], \quad (3.18d)$$

$$s_{k,m} \geq 0 \quad (k, m) \in \mathcal{I} \times [\mathcal{I}]. \quad (3.18e)$$

To derive first order optimality conditions, we discuss for a fixed parameter $\varepsilon > 0$ the differentiability of the control-to-state operator $S_O : U \times (-\varepsilon, \infty)^{\mathcal{I}} \rightarrow W(t_0, t_f)$, $(u, \alpha) \mapsto y$, where y is the unique solution to (3.9) for (u, α) .

Lemma 3.19. *The control-to-state operator S_O is continuously Fréchet-differentiable.*

Proof. We adapt the proof of [10, Lemma 4] to the present setting. We consider the mapping $e : W(t_0, t_f) \times U \times (-\varepsilon, \infty)^{\mathcal{I}} \rightarrow L^2_{[t_0, t_f]}(Z^*) \times H$ defined by

$$(y, u, \alpha) \mapsto e(y, u, \alpha) = (y_\tau - (\bar{\alpha} + \varepsilon) A y - (\bar{\alpha} + \varepsilon) F_{v_{\mathcal{M}}} u, y(t_0) - y_0).$$

For every $(y, u, \alpha) \in W(t_0, t_f) \times U \times (-\varepsilon, \infty)^{\mathcal{J}}$ the equality $S_O(u, \alpha) = y$ holds if and only if $e(y, u, \alpha) = 0$. We will demonstrate that e is continuously Fréchet-differentiable and the derivative $D_y e(y, u, \alpha)$ is onto for every (y, u, α) . Then, the claim is a consequence of the implicit function theorem. First, we note that the mappings

$$\begin{aligned} \mathcal{G}_1 : W(t_0, t_f) &\rightarrow L^2_{[t_0, t_f]}(Z^*), \quad y \mapsto y_\tau, & \mathcal{G}_2 : W(t_0, t_f) &\rightarrow L^2_{[t_0, t_f]}(Z^*), \quad y \mapsto Ay, \\ \mathcal{G}_3 : (-\varepsilon, \infty)^{\mathcal{J}} &\rightarrow L^\infty_{[t_0, t_f]}(\mathbb{R}), \quad \alpha \mapsto \bar{\alpha}, & \mathcal{G}_4 : U &\rightarrow U, \quad u \mapsto F_{v, \mathcal{H}} u, \\ \mathcal{G}_5 : W(t_0, t_f) &\rightarrow H, \quad y \mapsto y(t_0), \end{aligned}$$

are all well-defined, linear, and continuous. Consequently, they are continuously Fréchet-differentiable. Furthermore, the mapping

$$\mathcal{G}_6 : L^\infty_{[t_0, t_f]}(\mathbb{R}) \times L^2_{[t_0, t_f]}(Z^*) \rightarrow L^2_{[t_0, t_f]}(Z^*), \quad (h_1, h_2) \mapsto h_1 \cdot h_2.$$

is well-defined, bilinear, and continuous. Thus, it is continuously Fréchet-differentiable. Eventually, e is continuously Fréchet-differentiable as it can be expressed as

$$e(y, u, \alpha) = (\mathcal{G}_1(y) - \mathcal{G}_6(\mathcal{G}_3(\alpha) + \varepsilon, \mathcal{G}_2(y)) - \mathcal{G}_6(\mathcal{G}_3(\alpha) + \varepsilon, \mathcal{G}_4(u)), \mathcal{G}_5(y) - y_0).$$

We are left to demonstrate the surjectivity of $D_y e(y, u, \alpha)$ for every $(y, u, \alpha) \in W(t_0, t_f) \times U \times (-\varepsilon, \infty)^{\mathcal{J}}$. Let $\alpha \in L^\infty_{[t_0, t_f]}(Z^*)$ and $\gamma \in H$ be given, then the system

$$w_\tau(\tau) = (\bar{\alpha}(\tau) + \varepsilon)Aw(\tau) + \alpha(\tau) \quad \tau \in [t_0, t_f], \quad (3.19a)$$

$$w(t_0) = \gamma, \quad (3.19b)$$

has a unique solution $w \in W(t_0, t_f)$ according to Lemma 3.9. \square

After successfully establishing the Fréchet-differentiability of S_O , we require suitable representations of $(D_{\alpha_m} S_O)_{m \in [\mathcal{J}]}$ and $D_u S_O$. We proceed as in [10] and define the linear mapping $\mathcal{K} : L^2_{[t_0, t_f]}(Z^*) \rightarrow W(t_0, t_f)$, $\alpha \mapsto w$, where w solves (3.19) for $\gamma = 0$. This mapping is well-posed and continuous by Lemma 3.9. In addition, we consider the mapping $\mathcal{K}^* : L^2_{[t_0, t_f]}(Z^*) \rightarrow W(t_0, t_f)$, $\beta \mapsto q$, where q solves the backward system

$$\begin{aligned} -q_\tau(\tau) &= (\bar{\alpha}(\tau) + \varepsilon)Aq(\tau) + \beta(\tau) & \tau \in [t_0, t_f], \\ q(t_f) &= 0. \end{aligned}$$

The operators \mathcal{K} and \mathcal{K}^* are indeed adjoint since for all $f \in L^2_{[t_0, t_f]}(Z^*)$ and $g \in L^2_{[t_0, t_f]}(Z^*)$

$$\langle g, \mathcal{K}(f) \rangle_{L^2_{[t_0, t_f]}(Z^*), L^2_{[t_0, t_f]}(Z)} = \langle f, \mathcal{K}^*(g) \rangle_{L^2_{[t_0, t_f]}(Z^*), L^2_{[t_0, t_f]}(Z)}$$

holds. Hence, we obtain the representations $D_u S_O(u, \alpha)\underline{u}$ and $D_{\alpha_m} S_O(u, \alpha)\underline{\alpha}$

$$D_u S_O(u, \alpha)\underline{u} = \mathcal{K}((\bar{\alpha} + \varepsilon)F_{v, \mathcal{H}}\underline{u}), \quad (3.20a)$$

$$D_{\alpha_m} S_O(u, \alpha)\underline{\alpha} = \mathcal{K}(\chi_m(Ay + F_{v, \mathcal{H}}u)\underline{\alpha}), \quad (3.20b)$$

for $\underline{u} \in U$ and $\underline{\alpha} \in \mathbb{R}$, respectively. After demonstrating the differentiability of the control-to-state operator S_O , we discuss the reduced formulation of (3.18), which admits only finite

dimensional constraints

$$\begin{aligned} \inf_{\substack{u \in U, \\ s \in \mathbb{R}^{2\mathcal{J}}}} \quad & J_r(u, \alpha, s) := \frac{1}{2} \|\sqrt{\bar{\alpha}} + \varepsilon \cdot (S_O(u, \alpha) - \bar{y}_d)\|_U^2 + \frac{\gamma_u}{2} \|\sqrt{\bar{\alpha}} + \varepsilon \cdot u\|_U^2 \\ & + \frac{\gamma_s}{2} \|s\|_{\mathbb{R}^{2\mathcal{J}}}^2 + \gamma_{\text{EC}} J_{\text{EC}}(\alpha, s) + \gamma_{\text{MY}} J_{\text{MY}}(S_O(u, \alpha), s) \\ \text{s.t.} \quad & \Delta_M I = \sum_{j=1}^{\mathcal{N}} \alpha_{(i-1)\mathcal{N}+j} \quad i \in [\mathcal{M}], \quad (3.21a) \\ & \alpha_m \geq 0 \quad m \in [\mathcal{I}], \quad (3.21b) \\ & s_{k,m} \geq 0 \quad (k, m) \in \mathcal{S} \times [\mathcal{I}]. \quad (3.21c) \end{aligned}$$

Definition 3.20. Let $\varepsilon > 0$ and $\delta > 1$. We consider the Lagrange function $\mathcal{L} : U \times [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{J}} \times \mathbb{R}^{2\mathcal{J}} \times \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{2\mathcal{J}} \rightarrow \mathbb{R}$, $(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s)$ maps to

$$J_r(u, \alpha, s) + \sum_{i=1}^{\mathcal{M}} \lambda_{\Sigma, i} \left(\sum_{j=1}^{\mathcal{N}} \alpha_{(i-1)\mathcal{N}+j} - \Delta_M I \right) - \sum_{m=1}^{\mathcal{I}} \mu_{\alpha, m} \alpha_m - \sum_{k \in \mathcal{S}} \sum_{m=1}^{\mathcal{I}} \mu_{k, m} s_{k, m} \quad (3.22)$$

for multipliers $\lambda_{\Sigma}, \mu_{\alpha}, \mu_s^{\top} = (\mu_a, \mu_b)^{\top}$.

Definition 3.21. Let $(u, \alpha, s) \in U \times [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{J}} \times \mathbb{R}^{2\mathcal{J}}$ be an admissible point for (3.21). We define the adjoint state $p \in W(t_0, t_f)$ associated with $y = S_O(u, \alpha)$ by

$$p = \mathcal{K}^* \left((\bar{\alpha} + \varepsilon)(y - \bar{y}_d) + \gamma_{\text{MY}} \sum_{m=1}^{\mathcal{I}} \chi_{I_m} S^*(h_+(S(y), s_{b, m}) - h_-(S(y), s_{a, m})) \right). \quad (3.23)$$

Herein, the weak formulation for (3.23) is defined by

$$\begin{aligned} \int_{t_0}^{t_f} \langle -p_{\tau}(\tau), \varphi(\tau) \rangle_{Z^*, Z} d\tau &= \int_{t_0}^{t_f} (\bar{\alpha}(\tau) + \varepsilon) \langle A p(\tau), \varphi(\tau) \rangle_{Z^*, Z} + (\bar{\alpha}(\tau) + \varepsilon) \langle y(\tau) - \bar{y}_d(\tau), \varphi(\tau) \rangle_H \\ &+ \gamma_{\text{MY}} \sum_{m=1}^{\mathcal{I}} \chi_{I_m}(\tau) \langle h_+(S(y(\tau)), s_{b, m}) - h_-(S(y(\tau)), s_{a, m}), S(\varphi(\tau)) \rangle_H d\tau \quad \forall \varphi \in L^2_{[t_0, t_f]}(Z). \end{aligned}$$

We arrive at the succeeding KKT-system to characterize a candidate for optimality.

Theorem 3.22. Let $(u, \alpha, s) \in U \times [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{J}} \times \mathbb{R}^{2\mathcal{J}}$ be a local minimizer of (3.21). Then, there are Lagrange multipliers $(\lambda_{\Sigma}, \mu_{\alpha}, \mu_s) \in \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{2\mathcal{J}}$ with $\mu_s^{\top} = (\mu_a, \mu_b)^{\top}$ such that the following system of necessary optimality conditions is fulfilled

$$0 = \sum_{j=1}^{\mathcal{N}} \alpha_{(i-1)\mathcal{N}+j} - \Delta_M I \quad i \in [\mathcal{M}], \quad (3.24a)$$

$$0 \leq \alpha_m, \quad 0 \leq \mu_{\alpha, m}, \quad 0 = \alpha_m \cdot \mu_{\alpha, m} \quad m \in [\mathcal{I}], \quad (3.24b)$$

$$0 \leq s_{k, m}, \quad 0 \leq \mu_{k, m}, \quad 0 = s_{k, m} \cdot \mu_{k, m} \quad (k, m) \in \mathcal{S} \times [\mathcal{I}], \quad (3.24c)$$

$$0_U = D_u \mathcal{L}(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s), \quad (3.24d)$$

$$0_{\mathbb{R}^{\mathcal{I}}} = D_{\alpha} \mathcal{L}(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s), \quad (3.24e)$$

$$0_{\mathbb{R}^{2\mathcal{J}}} = D_s \mathcal{L}(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s), \quad (3.24f)$$

Proof. The presented problem can be interpreted as an abstract optimization problem in Banach spaces. We introduce the constraint mapping $\mathcal{G} : [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{I}} \times \mathbb{R}^{2\mathcal{I}} \rightarrow \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{\mathcal{I}}$

$$(\alpha, s) \mapsto \left(\left(\sum_{j=1}^{\mathcal{N}} \alpha_{(i-1)\mathcal{N}+j} - \Delta_{\mathcal{M}} I \right)_{i \in [\mathcal{M}]}, (-\alpha_m)_{m \in [\mathcal{I}]}, (-s_{a,m})_{m \in [\mathcal{I}]}, (-s_{b,m})_{m \in [\mathcal{I}]} \right)$$

together with the closed and convex cone $\mathcal{K} := 0_{\mathbb{R}^{\mathcal{M}}} \times [0, \infty)^{\mathcal{I}} \times [0, \infty)^{\mathcal{I}} \times [0, \infty)^{\mathcal{I}}$. Hence, we can write (3.21) with $\mathcal{C} := \mathcal{C}_u \times \mathcal{C}_\alpha \times \mathcal{C}_s$, $\mathcal{C}_u := U$, $\mathcal{C}_\alpha := [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{I}}$, and $\mathcal{C}_s := \mathbb{R}^{2\mathcal{I}}$ in the abstract form

$$\begin{aligned} & \inf_{(u, \alpha, s) \in \mathcal{C}} J_r(u, \alpha, s) \\ \text{s.t. } & \mathcal{G}(\alpha, s) \in -\mathcal{K}. \end{aligned}$$

To derive the optimality system, we check the well-known Robinson's CQ at (u, α, s) , which is given by

$$0 \in \text{Int}(\mathcal{G}(\alpha, s) + D\mathcal{G}(\alpha, s)((\mathcal{C}_\alpha \times \mathcal{C}_s) - (\alpha, s)) + \mathcal{K}). \quad (3.25)$$

For finite dimensional input (α, s) , Robinson's CQ is equivalent to the Mangasarian-Fromovitz CQ (MFCQ) [38]. MFCQ can be inferred from the stronger linear independence CQ (LICQ). Hence, it is sufficient to validate LICQ for our framework. The constraints on α , (3.21a) – (3.21b), and on s , (3.21c), are decoupled. Therefore, it is enough to verify LICQ individually for each set of constraints.

We start with the constraints on s . The Jacobian of (3.21c) with respect to s yields $-\text{Id}_{2\mathcal{I}}$. Here, Id_n denotes the identity matrix in $\mathbb{R}^{n \times n}$ for $n \in \mathbb{N}$. Hence, also the part matrix formed by the indices of the active constraints from (3.21c) is onto.

The Jacobian of (3.21a) – (3.21b) with respect to α again admits a block structure with regard to the major intervals. Hence, we can discuss LICQ individually for each major interval.

The part matrix of the Jacobian for the i -th major interval with $i \in [\mathcal{M}]$ is given by $\begin{pmatrix} \mathbf{1}_{\mathcal{N}}^\top \\ -\text{Id}_{\mathcal{N}} \end{pmatrix}$, which is not onto. Here, $\mathbf{1}_n \in \mathbb{R}^n$ denotes for $n \in \mathbb{N}$ the vector, which contains a one in each entry. However, in each major interval there can exist at most $\mathcal{N} - 1$ inactive minor intervals as each inactive minor interval corresponds to an active inequality constraint. Therefore, the part matrix formed by the indices of the active constraints from (3.21a) – (3.21b) is again onto. Consequently, LICQ is satisfied and (3.25) holds at (u, α, s) . Then, [27, Chapter 5.2 Theorem 5.3] ensures the existence of Lagrange multipliers $(\lambda_\Sigma, \mu_\alpha, \mu_s) \in \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{I}} \times \mathbb{R}^{2\mathcal{I}}$ such that the following optimality system is satisfied

$$0 = \sum_{j=1}^{\mathcal{N}} \alpha_{(i-1)\mathcal{N}+j} - \Delta_{\mathcal{M}} I \quad i \in [\mathcal{M}], \quad (3.26a)$$

$$0 \leq \alpha_m, \quad 0 \leq \mu_{\alpha, m}, \quad 0 = \alpha_m \cdot \mu_{\alpha, m} \quad m \in [\mathcal{I}], \quad (3.26b)$$

$$0 \leq s_{k, m}, \quad 0 \leq \mu_{k, m}, \quad 0 = s_{k, m} \cdot \mu_{k, m} \quad (k, m) \in \mathcal{I} \times [\mathcal{I}], \quad (3.26c)$$

$$0 \leq D\mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s)(\hat{u} - u, \hat{\alpha} - \alpha, \hat{s} - s) \quad (\hat{u}, \hat{\alpha}, \hat{s}) \in \mathcal{C}. \quad (3.26d)$$

To derive the statements in (3.24d) – (3.24f), we test the variational inequality (3.26d) successively with (\hat{u}, α, s) , $(u, \hat{\alpha}, s)$, and $(u, \alpha, \hat{s}) \in \mathcal{C}$.

□

Corollary 3.23. *Let $(u, \alpha, s) \in U \times [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{I}} \times \mathbb{R}^{2 \cdot \mathcal{I}}$ be a local minimizer of (3.21). The optimality conditions (3.24d) – (3.24f) of Theorem 3.22 can be expressed with the adjoint state p from Definition 3.21 as:*

$$0_H = (\bar{\alpha}(\tau) + \varepsilon)(\gamma_u u(\tau) + F_{v_{\mathcal{I}}}^*(\tau)p(\tau)), \quad (3.27)$$

for almost all $\tau \in [t_0, t_f]$.

$$\begin{aligned} 0 &= \frac{1}{2} \int_{I_m} \|S_O(u, \alpha)(\tau) - \bar{y}_d(\tau)\|_H^2 d\tau + \frac{\gamma_u}{2} \int_{I_m} \|u(\tau)\|_H^2 d\tau \\ &\quad - \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle S_O(u, \alpha)(\tau) - \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t \bar{\alpha}(\tau) d\tau \\ &\quad + \int_{I_m} \langle p(\tau), AS_O(u, \alpha)(\tau) + F_{v_{\mathcal{I}}}^*(\tau)u(\tau) \rangle_{Z, Z^*} d\tau \\ &\quad + \frac{\gamma_{EC}}{2} \sum_{k \in \mathcal{I}} D_{\alpha} \varphi_{FB}^2(\alpha_m, s_{k,m}) + \lambda_{\Sigma, i} - \mu_{\alpha, m}, \end{aligned} \quad (3.28)$$

for all $m \in [\mathcal{I}]$.

$$0 = \gamma_s s_{a,m} + \frac{\gamma_{EC}}{2} D_s \varphi_{FB}^2(\alpha_m, s_{a,m}) - \gamma_{MY} \int_{I_m} h_-(S(S_O(u, \alpha)), s_{a,m})(\tau) d\tau - \mu_{a,m}, \quad (3.29)$$

$$0 = \gamma_s s_{b,m} + \frac{\gamma_{EC}}{2} D_s \varphi_{FB}^2(\alpha_m, s_{b,m}) - \gamma_{MY} \int_{I_m} h_+(S(S_O(u, \alpha)), s_{b,m})(\tau) d\tau - \mu_{b,m}, \quad (3.30)$$

for all $m \in [\mathcal{I}]$.

Proof. With the help of the adjoint state p , we can derive pointwise statements for (3.24d) – (3.24f). We start with the evaluation of $D_u \mathcal{L}(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s) \underline{u}$ for $\underline{u} \in U$

$$\begin{aligned} D_u \mathcal{L}(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s) \underline{u} &= D_u J_r(u, \alpha, s) \underline{u} \\ &= \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle S_O(u, \alpha)(\tau) - \bar{y}_d(\tau), D_u S_O(u, \alpha)(\tau) \underline{u}(\tau) \rangle_H d\tau \\ &\quad + \gamma_u \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle u(\tau), \underline{u}(\tau) \rangle_H d\tau \\ &\quad + \gamma_{MY} \int_{[t_0, t_f]} \sum_{m=1}^{\mathcal{I}} \chi_{I_m}(\tau) h_+(S(S_O(u, \alpha)), s_{b,m})(\tau) S(D_u S_O(u, \alpha)(\tau) \underline{u}(\tau)) d\tau \\ &\quad - \gamma_{MY} \int_{[t_0, t_f]} \sum_{m=1}^{\mathcal{I}} \chi_{I_m}(\tau) h_-(S(S_O(u, \alpha)), s_{a,m})(\tau) S(D_u S_O(u, \alpha)(\tau) \underline{u}(\tau)) d\tau. \end{aligned} \quad (3.31)$$

From (3.31), the definition of p , and (3.20a) we conclude

$$\begin{aligned} D_u \mathcal{L}(u, \alpha, s, \lambda_{\Sigma}, \mu_{\alpha}, \mu_s) \underline{u} \\ = \gamma_u \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle u(\tau), \underline{u}(\tau) \rangle_H d\tau + \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle p(\tau), F_{v_{\mathcal{I}}}^*(\tau) \underline{u}(\tau) \rangle_H d\tau. \end{aligned}$$

We obtain (3.27) from (3.24d). We proceed with $D_{\alpha_m} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{\alpha}$ for $\underline{\alpha} \in \mathbb{R}$

$$\begin{aligned}
D_{\alpha_m} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{\alpha} &= D_{\alpha_m} J_r(u, \alpha, s) \underline{\alpha} + \lambda_{\Sigma, i} \underline{\alpha} - \mu_m \underline{\alpha} \\
&= \frac{1}{2} \int_{I_m} \underline{\alpha} \|S_O(u, \alpha)(\tau) - \bar{y}_d(\tau)\|_H^2 d\tau + \frac{\gamma_u}{2} \int_{I_m} \underline{\alpha} \|u(\tau)\|_H^2 d\tau \\
&\quad + \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle S_O(u, \alpha)(\tau) - \bar{y}_d(\tau), D_{\alpha_m} S_O(u, \alpha) \underline{\alpha} \rangle_H d\tau \\
&\quad - \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle S_O(u, \alpha)(\tau) - \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t \bar{\alpha}(\tau) \underline{\alpha} d\tau \\
&\quad + \gamma_{MY} \int_{[t_0, t_f]} \sum_{m=1}^{\mathcal{J}} \chi_{I_m}(\tau) h_+(S(S_O(u, \alpha)), s_{b,m})(\tau) S(D_{\alpha_m} S_O(u, \alpha)(\tau) \underline{\alpha}) d\tau \\
&\quad - \gamma_{MY} \int_{[t_0, t_f]} \sum_{m=1}^{\mathcal{J}} \chi_{I_m}(\tau) h_-(S(S_O(u, \alpha)), s_{a,m})(\tau) S(D_{\alpha_m} S_O(u, \alpha)(\tau) \underline{\alpha}) d\tau \\
&\quad + \frac{\gamma_{EC}}{2} \sum_{k \in \mathcal{S}} D_\alpha \varphi_{FB}^2(\alpha_m, s_{k,m}) \underline{\alpha} + \lambda_{\Sigma, i} \underline{\alpha} - \mu_{\alpha, m} \underline{\alpha}.
\end{aligned} \tag{3.32}$$

From (3.32), the definition of p , and (3.20b) we obtain

$$\begin{aligned}
D_{\alpha_m} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{\alpha} &= \frac{1}{2} \int_{I_m} \underline{\alpha} \|S_O(u, \alpha)(\tau) - \bar{y}_d(\tau)\|_H^2 d\tau + \frac{\gamma_u}{2} \int_{I_m} \underline{\alpha} \|u(\tau)\|_H^2 d\tau \\
&\quad - \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle S_O(u, \alpha)(\tau) - \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t \bar{\alpha}(\tau) \underline{\alpha} d\tau \\
&\quad + \int_{I_m} \langle (AS_O(u, \alpha)(\tau) + F_{v, \mathcal{H}}(u(\tau))) \underline{\alpha}, p(\tau) \rangle_{Z^*, Z} d\tau \\
&\quad + \frac{\gamma_{EC}}{2} \sum_{k \in \mathcal{S}} D_\alpha \varphi_{FB}^2(\alpha_m, s_{k,m}) \underline{\alpha} + \lambda_{\Sigma, i} \underline{\alpha} - \mu_m \underline{\alpha}.
\end{aligned}$$

Hence, we conclude (3.28) from (3.24e). We complete the calculation of derivatives with $D_{s_{a,m}} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{s}$ and $D_{s_{b,m}} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{s}$ for $\underline{s} \in \mathbb{R}$

$$\begin{aligned}
D_{s_{a,m}} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{s} &= \gamma_s s_{a,m} \underline{s} + \frac{\gamma_{EC}}{2} D_s \varphi_{FB}^2(\alpha_m, s_{a,m}) \underline{s} \\
&\quad - \gamma_{MY} \int_{I_m} h_-(S(S_O(u, \alpha)), s_{a,m})(\tau) \underline{s} d\tau - \mu_{a,m} \underline{s}, \\
D_{s_{b,m}} \mathcal{L}(u, \alpha, s, \lambda_\Sigma, \mu_\alpha, \mu_s) \underline{s} &= \gamma_s s_{b,m} \underline{s} + \frac{\gamma_{EC}}{2} D_s \varphi_{FB}^2(\alpha_m, s_{b,m}) \underline{s} \\
&\quad - \gamma_{MY} \int_{I_m} h_+(S(S_O(u, \alpha)), s_{b,m})(\tau) \underline{s} d\tau - \mu_{b,m} \underline{s}.
\end{aligned}$$

This yields with (3.24f) the conditions (3.29) – (3.30). \square

4. ALGORITHMIC DESIGN

In this section, we introduce our algorithmic approach to solve (3.21) by utilizing (3.9), (3.23), (3.24a) – (3.24c), and the corresponding pointwise formulations of (3.24d) – (3.24f), cf. Corollary 3.23. As intended, we apply the semismooth Newton method in function spaces, cf. [23]. For that purpose, we reformulate the equilibrium constraints (3.24b) – (3.24c) with a

suitable NCP function. We again employ φ_{FB} . We consider $M : W \rightarrow Z$,

$$W := W(t_0, t_f) \times U \times \left[-\frac{\varepsilon}{\delta}, \infty\right)^{\mathcal{J}} \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{\mathcal{J}} \times W(t_0, t_f) \times \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{\mathcal{J}}$$

with $x = (y, u, \alpha, s_a, s_b, p, \lambda_\Sigma, \mu_\alpha, \mu_a, \mu_b) \in W$. Similarly, we define the image space

$$Z := L^2_{[t_0, t_f]}(Z^*) \times H \times L^2_{[t_0, t_f]}(Z^*) \times H \times \mathbb{R}^{\mathcal{M}} \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{2\mathcal{J}} \times U \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{\mathcal{J}}.$$

Then, $M : W \rightarrow Z$ describes the nonlinear mapping, which contains the previously discussed optimality conditions (3.9), (3.23), (3.24a), (3.24b), (3.24c), (3.27), (3.28), (3.29), and (3.30) in ascending numerical order. The details on the involved derivatives can be found in Appendix A.

Algorithm. Set $k = 0$ and initialize $x_0 \in W$ together with the penalty parameters $\gamma_{\text{EC}}, \gamma_{\text{MY}} > 0$. Select tolerances $\text{Tol}_N, \text{Tol}_{\text{EC}}, \text{Tol}_{\text{MY}} > 0$ and updates $\delta_{\text{EC}}, \delta_{\text{MY}} > 1$.

```

while ( $\|M(x_k)\|_W \geq \text{Tol}_N$  or  $J_{\text{EC}}(\alpha_k, s_k) \geq \text{Tol}_{\text{EC}}$  or  $J_{\text{MY}}(y_k, s_k) \geq \text{Tol}_{\text{MY}}$ ) do
  while ( $\|M(x_k)\|_W \geq \text{Tol}_N$ ) do
    Select an element  $N \in \partial_G M(x_k)$ ;
    Solve  $N\delta d_k = -M(x_k)$  for  $\delta d_k$ ;
    Select step size  $t_k \in (0, 1]$ ;
    Project  $x_{k+1} = P_W(x_k + t_k \delta d_k)$ ;
    Update  $k = k + 1$ ;
  end
  if ( $J_{\text{EC}}(\alpha_k, s_k) \geq J_{\text{MY}}(y_k, s_k)$ ) then
    Update  $\gamma_{\text{EC}} = \gamma_{\text{EC}} \cdot \delta_{\text{EC}}$ ;
  else
    Update  $\gamma_{\text{MY}} = \gamma_{\text{MY}} \cdot \delta_{\text{MY}}$ ;
  end
end

```

Algorithm 1: Semismooth Newton with penalty homotopy.

The proposed algorithm consists of two main components. In the inner while-loop the optimality system is solved by the semismooth Newton method for a fixed pair of penalty parameters $(\gamma_{\text{EC}}, \gamma_{\text{MY}})$. After selection of an appropriate stepsize, the obtained point is projected onto W such that S_O can be evaluated. This procedure yields the next iterate x_{k+1} . In the subsequent if-block we adjust the parameters of the penalty homotopy according to the ratio of the violation of the penalized constraints. The algorithm terminates once the obtained residuum is less than a prescribed threshold Tol_N and selected tolerances $\text{Tol}_{\text{EC}}, \text{Tol}_{\text{MY}}$ on the penalized constraints are achieved.

Given a semismooth function $N : X \rightarrow Y$ between Banach spaces X and Y , we denote the generalized differential by $\partial_G N : X \rightrightarrows \mathcal{L}(X, Y)$. Hence, N is called $\partial_G N$ semismooth at $x \in X$ if

$$\sup_{J \in \partial_G N(x+d)} \|N(x+d) - N(x) - Jd\|_Y = o(\|d\|_X) \text{ for } \|d\|_X \rightarrow 0.$$

Algorithm 1 is typically only locally convergent. We attempt to heuristically increase the region of convergence by a suitable adjustment of the utilized step size. For that purpose, we

extend the cost function J_p to the merit function \mathcal{M} , which apart from the objective function also takes a feasibility term, weighted by a parameter $\gamma_F > 0$, into account.

First, we introduce the main part of the state and adjoint equation for a fixed $\varepsilon > 0$, $P_{\varepsilon, \pm} : W(t_0, t_f) \times [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{J}} \rightarrow L^2_{[t_0, t_f]}(Z^*)$, $(y, \alpha) \mapsto P_{\varepsilon, \pm}(y, \alpha)$. Consequently, the evaluation $P_{\varepsilon, \pm}$ is given by

$$P_{\varepsilon, \pm}(y, \alpha)(\varphi) = \int_{t_0}^{t_f} \langle \pm y_{\tau}(\tau) - (\bar{\alpha}(\tau) + \varepsilon)Ay(\tau), \varphi(\tau) \rangle_{Z^*, Z} d\tau \quad \forall \varphi \in L^2_{[t_0, t_f]}(Z).$$

Afterwards, we define the fidelity function $F : W(t_0, t_f) \times U \times [-\frac{\varepsilon}{\delta}, \infty)^{\mathcal{J}} \times \mathbb{R}^{2 \cdot \mathcal{J}} \rightarrow \mathbb{R}$, (y, u, α, s) maps to

$$\begin{aligned} F(y, u, \alpha, s) = & \left\| P_{\varepsilon, +}(y, \alpha) - (\bar{\alpha} + \varepsilon)F_{v_{\mathcal{M}}} u \right\|_{L^2_{[t_0, t_f]}(Z^*)} + \|y(0) - y_0\|_H + \|(-\alpha_m^+)_{m \in [\mathcal{J}]}\|_{\mathbb{R}^{\mathcal{J}}} \\ & + \sum_{k \in \mathcal{J}} \|(-s_{k, m}^+)_{m \in [\mathcal{J}]}\|_{\mathbb{R}^{\mathcal{J}}} + \left\| \left(\sum_{j=1}^{\mathcal{N}} \alpha_{(i-1) \cdot \mathcal{N} + j} - \Delta M I \right)_{i \in [\mathcal{M}]} \right\|_{\mathbb{R}^{\mathcal{M}}}. \end{aligned}$$

Then, we declare the merit function $\mathcal{M} : W(t_0, t_f) \times U \times \mathbb{R}^{\mathcal{J}} \times \mathbb{R}^{2 \cdot \mathcal{J}} \rightarrow \mathbb{R}$,

$$(y, u, \alpha, s) \mapsto \mathcal{M}(y, u, \alpha, s) = J_p(y, u, \alpha, s) + \gamma_F F(y, u, \alpha, s) \quad (4.1)$$

Furthermore, given a step size $t \in (0, 1]$ and search direction $\delta d \in W$, we define

$$\mathcal{M}_{t, \delta d}(y, u, \alpha, s) := \mathcal{M}(y + t\delta d_y, u + t\delta d_u, \alpha + t\delta d_\alpha, s + t\delta d_s).$$

Here, δd_\bullet denotes for $\bullet \in \{y, u, \alpha, s\}$ the vector, which consists only of the entries in δd corresponding to the selected variable.

Algorithm. Fix $\beta \in (0, 1)$ and $0 < \text{MaxIter} < \infty$. Initialize $k = 0$ and $t_0 = 1$.

```

while ( $\mathcal{M}_{t_k, \delta d}(y, u, \alpha, s) \geq \mathcal{M}(y, u, \alpha, s)$  and  $k < \text{MaxIter}$ ) do
  | Update  $t_{k+1} = t_k \cdot \beta$ ;
  | Update  $k = k + 1$ ;
end
if ( $\mathcal{M}_{t_k, \delta d}(y, u, \alpha, s) < \mathcal{M}(y, u, \alpha, s)$ ) then
  | Accept step width  $t = t_k$ ;
else
  | Reset step width  $t = 1$ ;
end

```

Algorithm 2: Globalization heuristic

Lastly, we also address the semismoothness of the involved superposition operators. The mappings $n_1 : \mathbb{R} \rightarrow \mathbb{R}$, $x \mapsto (x)_+$, $n_2 : \mathbb{R}^2 \rightarrow \mathbb{R}^2$, $(x, y) \mapsto \nabla \varphi_{\text{FB}}^2(x, y)$ both are globally Lipschitz continuous and semismooth functions [8]. Furthermore, the superposition mappings

$$\begin{aligned} N_- : W(t_0, t_f) \times \mathbb{R}^{\mathcal{J}} & \rightarrow L^2_{[t_0, t_f]}(\mathbb{R}), (y, s) \mapsto \left(a_{v_{\mathcal{M}}} - S(y) - \bar{s} \right)_+, \\ N_+ : W(t_0, t_f) \times \mathbb{R}^{\mathcal{J}} & \rightarrow L^2_{[t_0, t_f]}(\mathbb{R}), (y, s) \mapsto \left(S(y) - b_{v_{\mathcal{M}}} - \bar{s} \right)_+, \end{aligned}$$

are well-posed. Here, $\bar{s} \in L^\infty_{[t_0, t_f]}(\mathbb{R})$ is constructed from $s \in \mathbb{R}^{\mathcal{J}}$ similarly as $\bar{\alpha}$ from α . The claimed semismoothness then results from [23, Section 2.5.2, Theorem 2.13]. Here, the norm gap is bridged by the continuous embeddings $L^\infty_{[t_0, t_f]}(\mathbb{R}) \hookrightarrow L^p_{[t_0, t_f]}(\mathbb{R})$ for $2 \leq p < \infty$.

For alternative globalization strategies and rigorous convergence results for the semismooth Newton algorithm, we refer to, e.g., [23, Sections 2.4 & 2.5]. The convergence theory for the Moreau-Yosida penalization applied to pure state constraints is discussed in [22], while a differentiable penalty approach towards MPECs is topic of [24, 25]. However, a rigorous combined convergence analysis for the penalty parameters $\gamma_{\text{EC}}, \gamma_{\text{MY}}$ in the proposed algorithm is out of scope for this paper. Instead, we report on the results of our numerical experiments.

5. NUMERICAL RESULTS

In this section, we present numerical results for Algorithm 1 on an illustrative test instance, while the stepsize selection is conducted according to Algorithm 2. As a benchmark test, we attempt to numerically recover the solution to the state equation in Example 2.7 obtained for a desired control u_d . We consider the state domain $\Omega = (0, 1)$ and time interval $(t_0, t_f) = (0, 1)$. We employ the switching rule

$$C : L^2(\Omega) \rightarrow \{1, 2\}, y \mapsto \begin{cases} 1 & \text{if } \int_{\Omega} y(s) ds \leq 0.1, \\ 2 & \text{if } \int_{\Omega} y(s) ds > 0.1. \end{cases}$$

This means the switching threshold is given by $\sigma = 0.1$. Furthermore, we set the corresponding control domains to $\Omega_1 = (\frac{1}{6}, \frac{2}{6})$ and $\Omega_2 = (\frac{4}{6}, \frac{5}{6})$, respectively. The objective of experiment is to reconstruct the input $u_d \equiv 7.5$ by tracking the associated state in Example 2.7 for homogeneous initial conditions. Simulation of the state equation with the regularization parameter $r = 10^{-1}$ and u_d on an equidistant 108×108 grid by finite differences yields the desired state y_d , cf. Figure 2a. There occurs a unique switch around $\pi_d \approx 0.176$ from mode 1 to 2. Hence, the switching schedule is $S_d = \{(0, 1), (\pi_d, 2)\}$. We point out that the control regime is always truncated to the control domain of the active mode $d(t) \in [D]$. Therefore, the acting control is given by $u_{d,a}(x, t) = u_d(x, t) \cdot \chi_{\Omega_{d(t)}}(x)$.

We partition the time domain into $\mathcal{M} = 2$ major intervals and $\mathcal{N} = 3$ minor intervals of equal length. Hence, our partition operates in total with $\mathcal{S} = 6$ intervals. Taking again the integer control $v_{\mathcal{M}}^{\mathcal{N}}$ from Example 3.7, we obtain the desired vector $\alpha_d = (1.056, 1.944, 0, 0, 3, 0)$.

To solve the involved state equations, we apply finite differences on an equidistant grid. Here, Δ_x and Δ_t denote the corresponding gridwidths with respect to space and time, respectively. We solve both the state and adjoint equation with the implicit Euler-method.

The merit function \mathcal{M} in (4.1) measures the primal admissibility of the involved iterates and the associated cost. For our computations, we set the fidelity parameter to $\gamma_F = 1$.

We abort the inner while-loop, which contains the Newton iteration, once the condition $\|D\mathcal{L}\| < 10^{-5}$ is satisfied. For the penalty homotopy, we utilize $\text{Tol}_{\text{EC}} = \text{Tol}_{\text{MY}} = 10^{-8}$ and update with $\delta_{\text{EC}} = \delta_{\text{MY}} = 10^1$.

We initialize the algorithm for the regularization parameter $\varepsilon = r = 10^{-1}$ with the controls $u_{\text{in}}(x, t) = 2$ for all $(x, t) \in Q$, $\alpha_{\text{in}} = 1_6$, and $s_{\text{in}} = 10^{-9} \cdot 1_6$. The initial inputs for y_{in} and p_{in} are given by the solution of the state and adjoint equation, respectively, for the aforementioned controls and states. The initial input for the multipliers is $\lambda_{\Sigma} = 0_6$, $\mu_{\alpha} = 0_6$, $\mu_s = 10^{-9} \cdot 1_6$. Finally, we set the parameters in the cost function to $\gamma_u = 10^{-9}$, $\gamma_s = 10^{-6}$, and $\gamma_{\text{EC}} = \gamma_{\text{MY}} = 10^{-8}$.

In our computational experiment we employ the gridwidths $\Delta_x = \Delta_t \in [\frac{1}{36}, \frac{1}{108}]$ in Matlab on a Dell Latitude 5450 with 16 GB RAM and Intel Core Ultra 5 135U CPU. We do not incorporate

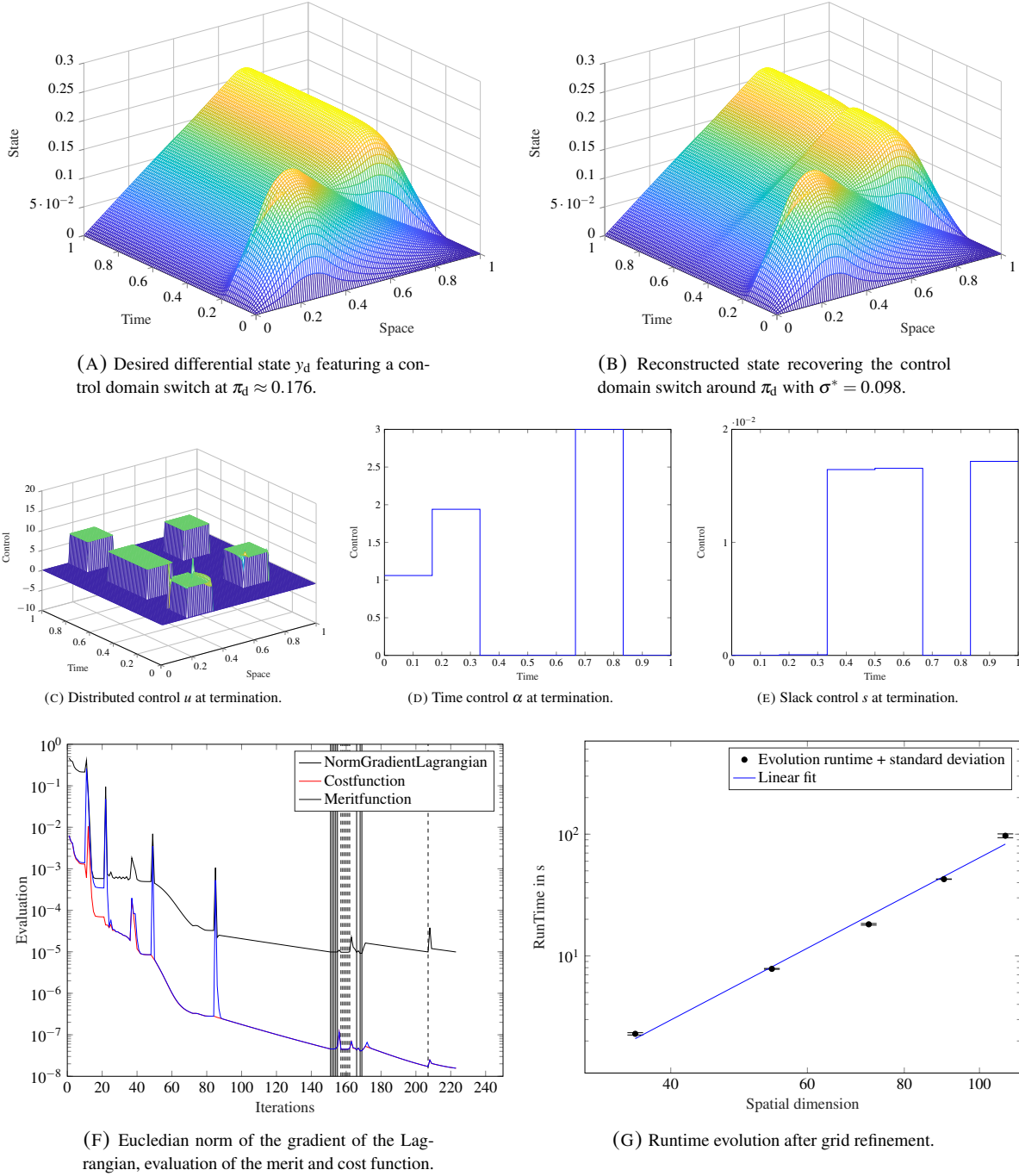


FIGURE 2. Numerical results for Example 2.7 on an equidistant 108×108 grid.

any external Matlab library or software package. The results presented in Figures 2a – 2g have been obtained for $\Delta_x = \Delta_t = \frac{1}{108}$.

In Figures 2a – 2b the desired state y_d , created by the control $u_{d,a}$, and the numerical reconstruction are presented. Both states result from the evaluation of the state equation in Example

2.7. The algorithmically reconstructed state in Figure 2b fits well to the desired state. In particular, the switch of the active control domain around time π_d is correctly recovered.

The Figures 2c – 2e depict the distributed control, time control, and slack after termination of the penalty homotopy, respectively. The obtained distributed control in Figure 2c corresponds well to the acting desired control $u_{d,a}$, while the calculated time control in Figure 2d matches with α_d . Overall, both controls $u_{d,a}$ and α_d are correctly recovered by the algorithm. The results on the slack control are illustrated in Figure 2e. On the active intervals, $m \in \{1, 2, 5\}$, the evaluation of the slack is marginal, while on the inactive intervals, $m \in \{3, 4, 6\}$, the slack compensates the violation of the switching rule.

The performance of the algorithm on the reported test instance during the penalty homotopy is displayed in Figure 2f. The cost and merit function gradually decrease over the runtime of the algorithm. The same is true for the norm of the gradient of the Lagrange function, which is capped by the threshold Tol_N . The occasional spikes of the merit function indicate points, where a non-decrease direction was accepted by Algorithm 2. The black vertical lines mark adjustments of the penalty parameter according to the update rule in the if-block of Algorithm 1. Herein, a dotted line indicates an increase of γ_{EC} , while a solid line marks an update of γ_{MY} . The algorithm terminates once all the tolerances Tol_{EC} and Tol_{MY} are satisfied. The indistinguishable difference between the cost and merit function indicates primal admissibility of the visited iterates.

In Figure 2g the computational effort is displayed for 15 inner iterations and various grid widths. The plot demonstrates that the runtime of the algorithm scales well in terms of grid refinement. The main computational effort during the inner iterations appears to be required by initialization and solution of the Newton system.

Altogether, the presented results underline the promising nature of the proposed algorithm. The reconstruction of $u_{d,a}$ and α_d are performed successfully. Based on a semismooth Newton method, the algorithm also displays a moderate increase in computational effort after grid refinement.

6. CONCLUSION

We presented a novel algorithmic approach to solve linear parabolic systems with an implicit switching mechanism. In the absence of a hybrid maximum principle, we combined techniques from the ODE framework, such as disjunctive programming and a time transformation method, with a penalization approach to derive a surrogate formulation, which was again eligible to a first optimize then discrete approach. During the various reformulation steps, we addressed the main adjustments and additional challenges within the PDE framework. This concerned in particular a regularization of the parabolic state equation, which we deemed necessary due to the appearance of an additional control term in the principal part of the state equation after application of the time transformation. As a consequence, the associated differential operator did no longer maintain a uniform ellipticity constant, which permitted the application of standard parabolic theory. Our main theoretical contributions range from a detailed convergence analysis for the regularized state equation up to the derivation of an optimality system for the surrogate formulation. However, a rigorous convergence study for the employed penalty approach was out of scope for this paper. Afterwards, the conducted numerical experiment underlined the promising nature of the proposed method on a newly introduced benchmark instance, where

the main objective was a precise detection of switching points. With the presented theoretical results, the proposed technique could pave the path for the proof a hybrid maximum principle with PDE dynamics. Future research projects could focus on the convergence analysis for the derived surrogate problem. Additionally, further numerical validation of the presented approach and the comparison to other reformulation approaches, e.g., Sum-Up-Rounding strategies [19] is desirable.

7. ACKNOWLEDGEMENTS

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APPENDIX A.

In this section, we elaborate the details on the computation of $\partial_G M$ from Section 4. Let $\mathcal{M} : \times_{i=1}^{n_X} X_i \rightarrow Y$ be a semismooth mapping for $n_X \in \mathbb{N}$. Furthermore, we consider for a fixed $\hat{x} \in \times_{i=1}^{n_X} X_i$ the mappings $\mathcal{M}_i : X_i \rightarrow Y, x \mapsto \mathcal{M}(\hat{x}_1, \dots, \hat{x}_{i-1}, x, \hat{x}_{i+1}, \dots, \hat{x}_{n_X})$, which are then also semismooth. Moreover, for every $i \in [n_X]$ we abbreviate $\partial_{G,i} \mathcal{M}(\hat{x}) := \partial_G \mathcal{M}_i(\hat{x}_i)$. In particular, we denote by $\partial_C \mathcal{M}$ Clarke's generalized differential, cf. [9].

First, we define $(h_m)_{m \in [\mathcal{J}]} := (h_1, \dots, h_m, \dots, h_{\mathcal{J}})^\top$. Herein, h_m is an element of a Banach space X for all $m \in [\mathcal{J}]$. Moreover, the notation $(h_{\tilde{m}})_{\tilde{m} \in [\mathcal{J}]}$ indicates that for $m \in [\mathcal{J}]$ exactly the m th entry of $(h_{\tilde{m}})_{\tilde{m} \in [\mathcal{J}]}$ is evaluated, while all remaining components are set to zero. Ultimately, the semismooth Newton method step for M can be formulated as

$$\begin{aligned} N(\delta y, \delta u, \delta \alpha, \delta s_a, \delta s_b, \delta p, \delta \lambda_\Sigma, \delta \mu_\alpha, \delta \mu_a, \delta \mu_b)^\top &= -M(y, u, \alpha, s_a, s_b, p, \lambda_\Sigma, \mu_\alpha, \mu_a, \mu_b), \\ N \in \partial_G M(y, u, \alpha, s_a, s_b, p, \lambda_\Sigma, \mu_\alpha, \mu_a, \mu_b). \end{aligned} \quad (\text{A.1})$$

Here, $N \in \mathcal{L}(W, Z)$ is row-wise declared in the following form. Note that we state only the non-zero contributions.

We begin with the derivative of the state equation (3.9)

$$\left[\begin{array}{c|c} D_y & P_{\varepsilon,+}(\cdot, \alpha) \\ D_u & -(\bar{\alpha} + \varepsilon) F_{v,\mathcal{N}} \\ D_\alpha & (-\chi_{I_m}(Ay + F_{v,\mathcal{N}}u))_{m \in [\mathcal{J}]} \end{array} \right]. \quad (\text{A.2})$$

We proceed with the derivative of the adjoint equation (3.23)

$$\left[\begin{array}{c|c} D_y & -(\bar{\alpha} + \varepsilon) \text{Id} + \gamma_{MY} \sum_{m=1}^{\mathcal{J}} \chi_{I_m} S^* (\partial_{C,1} h_-(S(y), s_{a,m}) - \partial_{C,1} h_+(S(y), s_{b,m})) S \\ D_\alpha & (-\chi_{I_m}(Ap + y - yd))_{m \in [\mathcal{J}]} \\ D_{s_a} & (\gamma_{MY} \chi_{I_m} S^* \partial_{C,2} h_-(S(y), s_{a,m}))_{m \in [\mathcal{J}]} \\ D_{s_b} & (-\gamma_{MY} \chi_{I_m} S^* \partial_{C,2} h_+(S(y), s_{b,m}))_{m \in [\mathcal{J}]} \\ D_p & P_{\varepsilon,-}(\cdot, \alpha) \end{array} \right]. \quad (\text{A.3})$$

Next, we provide for $i \in [\mathcal{M}]$ the derivative of the sum constraint (3.26a)

$$\left[D_\alpha \mid ((1)_{j \in [\mathcal{N}]})_{i \in [\mathcal{M}]}^i \right]. \quad (\text{A.4})$$

We continue for $m \in [\mathcal{J}]$ with the derivative of the complementarity condition on α and its corresponding Lagrange multiplier μ_α from (3.26b)

$$\left[\begin{array}{c|c} D_\alpha & (\partial_{C,1} \Phi_{FB}(\alpha_{\tilde{m}}, \mu_{\alpha,\tilde{m}}))_{\tilde{m} \in [\mathcal{J}]}^m \\ D_{\mu_\alpha} & (\partial_{C,2} \Phi_{FB}(\alpha_{\tilde{m}}, \mu_{\alpha,\tilde{m}}))_{\tilde{m} \in [\mathcal{J}]}^m \end{array} \right]. \quad (\text{A.5})$$

We state for $m \in [\mathcal{J}]$ the derivative of the complementarity condition on s and its associated Lagrange multipliers $\mu_{s,a}$ and $\mu_{s,b}$ from (3.26c)

$$\left[\begin{array}{c|c} D_{s_a} & (\partial_{C,1} \Phi_{FB}(s_{a,\tilde{m}}, \mu_{a,\tilde{m}}))_{\tilde{m} \in [\mathcal{J}]}^m \\ D_{\mu_a} & (\partial_{C,2} \Phi_{FB}(s_{a,\tilde{m}}, \mu_{a,\tilde{m}}))_{\tilde{m} \in [\mathcal{J}]}^m \end{array} \right], \left[\begin{array}{c|c} D_{s_b} & (\partial_{C,1} \Phi_{FB}(s_{b,\tilde{m}}, \mu_{b,\tilde{m}}))_{\tilde{m} \in [\mathcal{J}]}^m \\ D_{\mu_b} & (\partial_{C,2} \Phi_{FB}(s_{b,\tilde{m}}, \mu_{b,\tilde{m}}))_{\tilde{m} \in [\mathcal{J}]}^m \end{array} \right]. \quad (\text{A.6})$$

We proceed with the derivative of (3.27), where $F_{v_{\mathcal{M}}}^* : H \rightarrow H$ is the adjoint operator to $F_{v_{\mathcal{M}}}$,

$$\begin{bmatrix} D_u & | & (\bar{\alpha} + \varepsilon)\gamma_u \text{Id} \\ D_\alpha & | & (\mathcal{X}_m(\gamma_u u + F_{v_{\mathcal{M}}}^* p))_{m \in [\mathcal{J}]} \\ D_p & | & (\bar{\alpha} + \varepsilon)F_{v_{\mathcal{M}}}^* \end{bmatrix}. \quad (\text{A.7})$$

Next, we discuss the derivative of (3.28) for $m \in [\mathcal{J}]$.

$$\begin{bmatrix} D_y & | & \int_{I_m} \langle (y(\tau) - \bar{y}_d(\tau)) - (\bar{\alpha}(\tau) + \varepsilon)D_t \bar{y}_d(\tau) D_{\alpha_m} t_{\bar{\alpha}}(\tau) + Ap(\tau), \cdot \rangle_{Z^*, Z} d\tau \\ D_u & | & \int_{I_m} \langle \gamma_u u(\tau) + F_{v_{\mathcal{M}}}^*(\tau)p(\tau), \cdot \rangle_H d\tau \\ D_\alpha & | & \begin{aligned} & \left(- \int_{I_m} \langle y(\tau) - \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t_{\bar{\alpha}}(\tau) d\tau \right. \\ & \quad - \int_{I_m} \langle y(\tau) - \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t_{\bar{\alpha}}(\tau) d\tau \\ & \quad + \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle D_t \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t_{\bar{\alpha}}(\tau) D_{\alpha_m} t_{\bar{\alpha}}(\tau) d\tau \\ & \quad - \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle y(\tau) - \bar{y}_d(\tau), D_{tt}^2 \bar{y}_d(\tau) \rangle_H D_{\alpha_m} t_{\bar{\alpha}}(\tau) D_{\alpha_m} t_{\bar{\alpha}}(\tau) d\tau \\ & \quad \left. - \int_{[t_0, t_f]} (\bar{\alpha}(\tau) + \varepsilon) \langle y(\tau) - \bar{y}_d(\tau), D_t \bar{y}_d(\tau) \rangle_H D_{\alpha_m}^2 t_{\bar{\alpha}}(\tau) d\tau \right. \\ & \quad \left. + \frac{\gamma_{EC}}{2} \sum_{k \in \mathcal{J}} \partial_{C,1} D_\alpha \Phi_{FB}^2(\alpha_{\bar{m}}, s_{k, \bar{m}}) \right)_{\bar{m} \in [\mathcal{M}]} \\ D_{s_a} & | & \left(\frac{\gamma_{EC}}{2} \partial_{C,2} D_\alpha \Phi_{FB}^2(\alpha_{\bar{m}}, s_{a, \bar{m}}) \right)_{\bar{m} \in [\mathcal{J}]}^m \\ D_{s_b} & | & \left(\frac{\gamma_{EC}}{2} \partial_{C,2} D_\alpha \Phi_{FB}^2(\alpha_{\bar{m}}, s_{b, \bar{m}}) \right)_{\bar{m} \in [\mathcal{J}]}^m \\ D_p & | & \int_{I_m} \langle Ay(\tau) + F_{v_{\mathcal{M}}}(\tau)u(\tau), \cdot \rangle_{Z^*, Z} d\tau \\ D_{\lambda_\Sigma} & | & (1)_{i \in [\mathcal{M}]}^i \\ D_{\mu_\alpha} & | & (-1)_{\bar{m} \in [\mathcal{J}]}^m \end{aligned} \end{bmatrix}. \quad (\text{A.8})$$

Eventually, we calculate the derivative of (3.29) and (3.30) for $m \in [\mathcal{J}]$

$$\begin{bmatrix} D_y & | & -\gamma_{MY} \int_{I_m} \langle S^* \partial_{C,1} h_-(S(y), s_{a,m})(\tau), \cdot \rangle_H d\tau \\ D_\alpha & | & \left(\frac{\gamma_{EC}}{2} \partial_{C,1} D_s \Phi_{FB}^2(\alpha_{\bar{m}}, s_{a, \bar{m}}) \right)_{\bar{m} \in [\mathcal{J}]}^m \\ D_{s_a} & | & \begin{aligned} & \left(\gamma_s + \frac{\gamma_{EC}}{2} \partial_{C,2} D_s \Phi_{FB}^2(\alpha_{\bar{m}}, s_{a, \bar{m}}) \right. \\ & \quad \left. - \gamma_{MY} \int_{I_m} \partial_{C,2} h_-(S(y), s_{a, \bar{m}})(\tau) d\tau \right)_{\bar{m} \in [\mathcal{J}]}^m \\ D_{\mu_a} & | & (-1)_{\bar{m} \in [\mathcal{J}]}^m \end{aligned} \end{bmatrix}, \quad (\text{A.9})$$

$$\begin{bmatrix} D_y & | & -\gamma_{MY} \int_{I_m} \langle S^* \partial_{C,1} h_+(S(y), s_{b,m})(\tau), \cdot \rangle_H d\tau \\ D_\alpha & | & \left(\frac{\gamma_{EC}}{2} \partial_{C,1} D_s \Phi_{FB}^2(\alpha_{\bar{m}}, s_{b, \bar{m}}) \right)_{\bar{m} \in [\mathcal{J}]}^m \\ D_{s_b} & | & \begin{aligned} & \left(\gamma_s + \frac{\gamma_{EC}}{2} \partial_{C,2} D_s \Phi_{FB}^2(\alpha_{\bar{m}}, s_{b, \bar{m}}) \right. \\ & \quad \left. - \gamma_{MY} \int_{I_m} \partial_{C,2} h_+(S(y), s_{b, \bar{m}})(\tau) d\tau \right)_{\bar{m} \in [\mathcal{J}]}^m \\ D_{\mu_b} & | & (-1)_{\bar{m} \in [\mathcal{J}]}^m \end{aligned} \end{bmatrix}. \quad (\text{A.10})$$