Bang-Bang and Singular Controls in Optimal Control Problems with Partial Differential Equations

Hans Josef Pesch, Simon Bechmann, and Jan-Eric Wurst

Abstract—This paper focuses on bang-bang and singular optimal controls for problems involving partial differential equations. In particular, singular controls have hardly ever been investigated in literature. Since existence of solutions and multipliers, as well as their regularity, cannot be proven in general for problems of this type, the derivation of candidates for necessary conditions via the so-called formal Lagrange technique seems to be the only viable way. Nevertheless, a numerical a posteriori verification of these conditions may fill this gap, at least to a certain extent. Finally, a generalization of a numerical method is presented, a counterpart of which has turned out to be efficient and robust for optimal control problems involving ordinary differential equations. This method allows a precise determination of the switches from one control type to the other, while the number of discrete optimization variables is considerably reduced.

I. INTRODUCTION

Bang-bang and singular controls are typical phenomena in optimal control problems of ordinary differential equations (OC-ODE) when the controls enter both the objective functional and the constraints linearly. While theory and numerics of these problems have been well-studied, so far only bang-bang controls have been investigated in optimal control of partial differential equations (OC-PDE) with the one exception of the not-easily accessible dissertation of Theißen [37]. Besides examples of elliptic and parabolic optimal control problems, where singular controls occur if integrands of tracking type functionals vanish in subdomains, the control of stationary states of nonlinear evolution equations is detected as another case where optimal controls can become singular.

Current research in OC-ODE deals with sufficient conditions for bang-bang (Agrachev et al. [1], Maurer, Osmolovskii [28], [29], [30], Milyutin, Osmolovskii [32], and Osmolovskii, Maurer [33], [34]), purely singular (Dmitruk [9], [10]), and bang-singular controls (Aronna [2], Dmitruk [11], [12]). Sufficiency conditions for general switching structures have not been developed so far. The best attempt to the solution of this still open problem is given by Vossen’s thesis [43], where a numerical method has been developed to verify sufficient conditions approximately.

In contrast, Tikhonov techniques are imposed in OC-PDE in order to proof existence, (local) uniqueness, and sufficient regularity of multipliers. However, this regularization technique prevents bang-bang and singular controls even if the controls otherwise enter the problems linearly. Apart from Theißen’s thesis [37], only pure bang-bang controls have been investigated in OC-PDE. Most of these publications date back many years: Bergounioux and Tröltzsch [3], Eppler and Tröltzsch [13], Glashoff and Sachs [18], Glashoff and Weck [19], Karafiat [20], Knowles [23], Mackenroth [25], Schmidt [36], Tröltzsch [38], [39], [40], [41], and more recently Deckelnick and Hinze [8]. The last reference deals with error estimates for discretization methods in case of bang-bang controls. Numerical experiments for elliptic optimal control problems with bang-bang controls have also been conducted by Maurer and Mittelmann [27].

Concerning numerical methods for OC-ODE, it has turned out that indirect, i.e., adjoint-based methods are extremely difficult to handle if problems are highly nonlinear and possess complicated switching structures; see, e.g., Bulirsch et al. [6]. Any deeper analysis of those problems is hampered by their intrinsic nonlinearity and, with regard to bang-singular subarcs, the difficulty of their detection; see again [6]. Therefore, in Fraser-Andrews [15], [16] and Bueskens et al. [5] postprocessing techniques have been developed to improve the accuracy of approximate solutions obtained by NLP methods according to the First-Optimize-Then-Discretize (FODT) approach (FODT). The idea is to transcribe the OC-ODE as a switching point optimization problem and to use a prescribed switching structure based on the evaluation of the previously computed NLP results and their coincidence with the optimal control law according to the minimum principle. Thereafter, necessary and even sufficient conditions for local optimal solutions can be approximately verified even for problems that would be hardly computable by indirect methods via the First-Optimize-Then-Discretize approach (FOTD); see, e.g., Maurer and Pesch [31] and Vossen [43].

The FDTO approach has also become popular in PDE constrained optimization; see, e.g., again [27] and Petit et. al. [35], and for a complicated engineering application on the fuel cell optimization (Chudej et. al. [7]).

The intention of this paper is to focus on bang-bang and singular optimal controls in OC-PDE. The derivation of necessary conditions by the so-called formal Lagrange technique (Tröltzsch [42]) is particularly justified for these problems since any deeper analysis concerning existence, (local) uniqueness and regularity seems to be hardly obtainable in general. Hence, we have to rely on numerical approximations. A further intention is to build bridges from...
OC-ODE to OC-PDE to develop new numerical methods for OC-PDE whose counterparts have already turned out to be efficient, precise and robust for OC-ODE.

II. SINGULAR CONTROL IN AN ELLIPTIC OPTIMAL CONTROL PROBLEM OF GRADIENT TRACKING TYPE

The following problem is motivated by the well-known van der Pol oscillator which is a prototype problem with pure bang-bang optimal control in the minimum time case (Kaya, Noakes [21], [22], Maurer, Osmolovski [28], [29]) and of bang-singular type for minimum damping while terminal time is specified (Vossen [43], [44]).

A. The “minimum-time elliptic van der Pol oscillator”

The following problem transfers the characteristic properties of the minimum-time control of the van der Pol oscillator to a semi-linear elliptic control problem with a distributed control. It is of purely academic nature and shall only serve to a semi-linear elliptic control problem with a distributed control. It is of purely academic nature and shall only serve as an example for demonstration purposes.

Let be \( \Omega := (0, T)^2 \), with \( T > 0 \) unspecified. The boundary \( \Gamma \) of \( \Omega \) shall be partitioned as follows: \( \Gamma = \Gamma_{SW} \cup \Gamma_{NE} \) with \( \Gamma_{SW} := \{(x, y), \, x \in [0, T]\} \cup \{(0, y), \, y \in [0, T]\} \) and \( \Gamma_{NE} := \{(x, T), \, x \in [0, T]\} \cup \{(T, y), \, y \in [0, T]\} \).

On \( \Omega \) the following semi-linear elliptic optimal control problem is defined, also interpretable as a simple shape optimization problem:

\[
\min J(z, v, T) = \min_{|v| \leq 1, \, T > 0} T + \frac{\varepsilon}{2} \int_{\Gamma_{NE}} (z - r)^2 \, ds,
\]

with \( \varepsilon > 0 \), subject to

\[
- \Delta z + (1 - z^2) (z_x + z_y) - z = v \quad \text{on} \quad \Omega,
\]

\[
z = 0 \quad \text{and} \quad \partial_v z = 1 \quad \text{on} \quad \Gamma_{SW},
\]

\[
\partial_v z = 0 \quad \text{on} \quad \Gamma_{NE}.
\]

The set of admissible controls is given by \( U_{ad} := \{v \in L^2(\Omega) : \, -1 \leq v \leq 1 \text{ a.e.}\} \), and \( r \) shall be constant, \( r = 0.2 \). Here, the symbol \( \Delta \) denotes the Laplace operator and subscripts partial derivatives. Later on, we will also use the symbol \( \nabla \) for the gradient and \( \partial_v \) for the derivative in the direction of the outward normal unit vector.

Due to the nonlinearity of the problem existence, uniqueness, and regularity results seem to be hardly provable. Therefore, we have to restrict ourselves to derive potential necessary conditions solely formally by the Lagrange technique and define the weak form of the Lagrangian as follows:

\[
\mathcal{L}(z, p, v, T) = T + \frac{\varepsilon}{2} \int_{\Gamma_{NE}} (z - r)^2 \, ds
\]

\[
- \int_{\Omega} \nabla z \cdot \nabla p + [(1 - z^2) (z_x + z_y)]
\]

\[
- z - v \, p \, dx \, dy + \int_{\Gamma_{SW}} p \, ds.
\]

Here the two Neumann boundary conditions have been built-in, while the Dirichlet boundary conditions have to be taken into account in the space of test functions later on. Note that the boundary integrals implicitly depend on the free “terminal time” \( T \).

Differentiation of \( \mathcal{L} \) with respect to the control \( v \) in the direction of admissible variations \( v - \bar{v} \) leads to the variational inequality, which determines the optimal control \( \bar{v} \):

\[
\mathcal{L}_v(z, p, \bar{v}, T) = (p, v - \bar{v})_{L^2(\Omega)} \geq 0 \quad \forall \, v \in U_{ad}
\]

with bars denoting optimal candidates and \( \langle \cdot, \cdot \rangle_{L^2(\Omega)} \) the scalar product in the Hilbert space \( L^2(\Omega) \). This variational inequality implies a pointwise control law for the optimal control \( \bar{v} \):

\[
\bar{v} = \begin{cases} 
-1 & \text{if} \quad p > 0, \\
\tau_{\text{sing}} & \text{if} \quad p \equiv 0, \\
+1 & \text{if} \quad p < 0.
\end{cases}
\]

Here the adjoint state \( p \) plays the role of a switching function.

Differentiation of \( \mathcal{L} \) with respect to the state variable \( z \) and \( \mathcal{L}_z(z, p, \bar{v}, T) = 0 \) lead, after some longer calculations and using the typical variational argument, to the adjoint equation

\[
- \Delta p - (1 - z^2) (p_x + p_y) - p = 0 \quad \text{on} \quad \Omega,
\]

\[
\partial_v p + (1 - z^2) = \varepsilon (z - r) \quad \text{on} \quad \Gamma_{NE}.
\]

It should be noted that a PDE is always to be understood in its weak form throughout this paper.

For the derivation of the necessary condition for the open boundary \( T \), we formally apply Leibniz’s rule and obtain

\[
\frac{d}{dT} \mathcal{L}(z, p, \bar{v}, T) = 1 - \int_0^T \dot{z}_{yy} p \vert (x, T) \, dx
\]

\[
- \int_0^T \dot{z}_{xx} p \vert (T, y) \, dy + \varepsilon (z(T, T) - r)^2 = 0.
\]

Note the typical form of transversality condition known from the maximum principle of OC-ODE.

For the ODE version of the minimum-time van der Pol oscillator, it can be easily proven that only bang-bang controls occur. The proof goes, as usual, by contradiction: the maximum principle requires not simultaneously vanishing multipliers. A proof for the PDE version remains open. Numerical results would be beyond the scope of this paper.

B. The minimum damping “elliptic van der Pol oscillator”

Let \( \Omega := (0, T)^2 \) now be equipped with a fixed “terminal time” \( T = \text{const} > 0 \). The boundary \( \Gamma \) of \( \Omega \) shall be partitioned as follows: \( \Gamma = \Gamma_N \cup \Gamma_E \cup \Gamma_S \cup \Gamma_W \) with \( \Gamma_N := \{(x, T), \, x \in [0, T]\}, \Gamma_E := \{(T, y), \, y \in [0, T]\}, \Gamma_S := \{(x, 0), \, x \in [0, T]\} \text{ and } \Gamma_W := \{(0, y), \, y \in [0, T]\} \). Furthermore we denote, e.g., by \( \Gamma_{NS} = \Gamma_N \cup \Gamma_S \).

Now we minimize the damping functional

\[
J(z, v) = \frac{1}{2} \int_\Omega z^2 + \dot{z}_x^2 + \dot{z}_y^2 \, dx \, dy
\]
subject to
\[- \Delta z + (1 - z^2) (z_x + z_y) - z = v \quad \text{on } \Omega ,\]
\[
\partial_\nu z = 0 \quad \text{on } \Gamma_{NES} ,
\]
\[
z = 0 \quad \text{and } \partial_\nu z = 1
\]
on \Gamma_W \cap \{(0, y) : 0.4 \leq y \leq 0.6\}

with the same set of admissible controls as before.

Using again the formal Lagrange technique the same control law is obtained, but the adjoint differential equation reads as follows
\[- \Delta p - \left(1 - \bar{z}^2\right) (p_x + p_y) - p = \Delta \bar{z} - \bar{z} \quad \text{on } \Omega .\]

The boundary conditions are omitted here, since they are neither needed for the further analysis nor for the FDTO method used in this paper.

In case of \( p \equiv 0 \) on a non-empty set \( \omega \subset \Omega \) of positive measure, the identity \( p \equiv 0 \) hides the additional identities \( \nabla p \equiv 0 \) and \( \Delta p \equiv 0 \). Then the adjoint differential equation together with the state equation yields the typical feedback form of a singular control on \( \omega \), if it exists at all,
\[v_{\text{sing}} := \left(1 - \bar{z}^2\right) (\bar{z}_x + \bar{z}_y) - 2 \bar{z} .\]

The subdomain where the control is singular is an analogue to a first-order singular subarc in OC-ODE, since here we have to apply a second-order differential operator to bring the singular control to light.

The following numerical results have been obtained by the FDTO approach, i.e., by transcribing the infinite dimensional problem into a finite dimensional nonlinear programming problem via the modelling language AMPL ([14]) and by using the interior point nonlinear programming solver IPOPT ([45]). Due to automatic differentiation provided by AMPL the NLP solver IPOPT can rely on first- and second-order gradient information making this approach not only convenient for unaware users, but also efficient for problems of moderate size. It is known that FDTO often abuts on its limits concerning the number of optimization variables. Therefore, in Subsection IV a generalization of the switching point optimization technique of OC-ODE is presented which may allow a considerable reduction of the number of optimization variables, if certain assumptions apply.

Figures 1–4 show the approximate candidate optimal solution of the damped problem. Figure 2 shows a bang-bang-singular switching structure of the optimal control. In Fig. 3 the difference between the optimal control \( \bar{v} \) and the feedback formula for the singular control \( v_{\text{sing}} \) clearly supports the above analysis, which moreover is certified by the adjoint state \( p \) vanishing in the singular subdomain; see Fig. 4. Note that the discrete adjoint provided by IPOPT has the opposite sign to the notation used throughout this paper. Herewith the main necessary conditions are numerically verified.

It should be emphasized that adjoint-based methods, resp. \textit{First Optimize Then Discretize} seem to be hardly applicable when singular domains occur. As in OC-ODE the usual junction between bang-bang and singular domains (besides
the rare continuously differentiable junction; Maurer [26]) seems to be present here, too. The smooth transition, which can be seen here, is most probably an unwanted numerical side-effect. In Subsection IV we will show how one can clarify the junction by a postprocessing step, if certain assumptions apply.

We now turn to a problem of practical interest where the junction can be precisely resolved.

III. SINGULAR CONTROL IN A HYPERBOLIC OPTIMAL CONTROL PROBLEM OF GRADIENT TRACKING TYPE

In Kunisch, Wachsmuth [24] a time-optimal control problem for the wave equation is analyzed. It reads as follows

$$\min J(y, u, t_f) = \min_{u \in U_{ad}} t_f$$

subject to

$$y_{tt}(x, t) - y_{xx}(x, t) = u(x, t) \text{ in } \Omega \times (0, t_f),$$

$$y(x, 0) = y_1(x) \quad \text{ in } \Omega,$$

$$y(x, 0) = y_2(x) \quad \text{ in } \Omega,$$

$$y(0, t) = 0 \quad \text{ in } [0, t_f],$$

$$y(1, t) = 0 \quad \text{ in } [0, t_f],$$

$$y(x, t_f) = z_1(x) \quad \text{ in } \Omega,$$

$$y_t(x, t_f) = z_2(x) \quad \text{ in } \Omega$$

with $\Omega = (0, 1)$. The set of admissible controls is given by $U_{ad} := \{ u \in L^2(\Omega \times (0, t_f)) : \| u(\cdot, t) \|_{L^2(\Omega)} \leq \gamma \ \text{a.e. in } (0, t_f) \}$ with $\gamma = \text{const} > 0$. It constitutes a control variable inequality, pointwise in time.

In Ref. [24] the authors show that this problem has a solution, if at all there is a control $u$ which steers the states $y_1$, $y_2$ to the terminal states $z_1$, $z_2$. Moreover, the minimum final time is unique. The basic idea of this paper is to regularize the control, to penalize the terminal conditions, and finally to show the convergence of the solution of the regularized and penalized problem to the solution of the original minimum-time problem. In addition, a complete regularity analysis has been developed. It turns out that the optimal solution is purely bang-bang which is the usual case in time-optimal control of OC-ODE, too.

A. The regularized minimum-time optimal control problem for the wave equation

We receive this problem here to demonstrate, on the one hand, the usage of the Lagrange technique, on the other hand, to correct the terminal time condition of [24] and start with the regularized, but not, as in [24], penalized objective

$$\min J(y, u, t_f) = \min_{u \in U_{ad}, \epsilon > 0} t_f + \frac{\lambda}{2} \| u \|_{L^2(\Omega \times (0, t_f))}^2$$

with $\lambda \geq 0$. Let us now begin with the strong version of the Lagrangian, where we adjoin all constraints by separate multipliers $(p, \alpha, \beta, \tilde{\beta}, \varrho, \phi = L, R)$, and perform partial integrations with respect to space and time

$$L(y, p, u, t_f) = t_f - \int_{t=0}^{t_f} \int_{x=0}^{1} (y_{tt} - y_{xx} - u) \, p \, dx \, dt + \frac{\lambda}{2} \int_{t=0}^{t_f} \int_{x=0}^{1} u^2 \, dx \, dt + \int_{x=0}^{1} (y(x, 0) - y_1(x)) \alpha(x) \, dx$$

$$+ \int_{x=0}^{1} (y(x, 0) - y_2(x)) \tilde{\beta}(x) \, dx + \int_{t=0}^{t_f} y(0, t) \varrho_L(t) \, dt$$

$$+ \int_{t=0}^{t_f} y(1, t) \varrho_R(t) \, dt + \int_{x=0}^{1} (y(x, t_f) - z_1(x)) \beta(x) \, dx$$

$$+ \int_{x=0}^{1} (y_t(x, t_f) - z_2(x)) \tilde{\beta}(x) \, dx$$

$$= t_f + \frac{\lambda}{2} \int_{t=0}^{t_f} \int_{x=0}^{1} u^2 \, dx \, dt$$

$$- \int_{x=0}^{1} y_t(x, t_f) \left( p(x, t_f) - \beta(x) \right) - y_t(x, 0) \left( p(x, 0) + \tilde{\beta}(x) \right) \right) \, dx$$

$$+ \int_{x=0}^{1} y(x, 0) - y_1(x) \right) \alpha(x) \, dx$$

$$- \int_{x=0}^{1} y_2(x) \tilde{\beta}(x) \, dx$$

$$+ \int_{t=0}^{t_f} y(0, t) \varrho_L(t) \, dt$$

$$+ \int_{t=0}^{t_f} y(1, t) \varrho_R(t) \, dt + \int_{x=0}^{1} (y(x, t_f) - z_1(x)) \beta(x) \, dx$$

$$- \int_{x=0}^{1} z_2(x) \tilde{\beta}(x) \, dx .$$

Differentiation with respect to the state $y$ and additional partial integrations with respect to space and time lead, by means of usual variational arguments, to the following adjoint system

$$- p_{tt} + p_{xx} = 0 \quad \text{on } \Omega \times (0, t_f),$$

$$p(0, t) = p(1, t) = 0 \quad \text{in } [0, t_f].$$

1Henceforth, the bar indicating optimal candidates is omitted unless it is absolutely necessary.
In addition, there follows
\[ p(x, 0) = -\tilde{\alpha}(x), \quad p_t(x, 0) = \alpha(x), \]
\[ p(x, t_f) = \tilde{\beta}(x), \quad p_t(x, t_f) = -\beta(x), \]
\[ p_x(0, t) = -q_L(t), \quad p_x(1, t) = q_R(t). \]
We observe that certain traces of the adjoint state and its derivatives coincide with the multipliers for the initial and boundary conditions. Note that we do not get initial conditions for the adjoint state \( p \) in \( t = t_f \) due to the prescribed terminal conditions for the state \( y \). Indeed it would be sufficient to take into account only the latter ones in the Lagrangian; the other conditions can alternatively be embedded in the space of test functions. Differentiation with respect to the control \( u \) yields
\[ D_u \mathcal{L}(\ddot{y}, p, \bar{u}, \bar{t}_f)(u - \bar{u}) = \int_{t=0}^{t_f} \left( \lambda \bar{u} + p \right) (u - \bar{u}) \, dx \, dt \geq 0 \quad \forall u \in U_{\text{ad}}, \]
resp. the projection formula
\[ \bar{u} = P_{U_{\text{ad}}} \left\{ -\frac{1}{\lambda} p \right\}. \]
Here, the projection \( P_{U_{\text{ad}}} \) has to be understood as follows: if
\[ \frac{1}{\lambda} \| p(\cdot, t) \|_{L^2(\Omega)} < \gamma, \]
define the optimal control \( \bar{u} := -\frac{1}{\lambda} p \). Otherwise determine a time-dependent scaling factor \( \kappa(t) \), such that
\[ \frac{1}{\lambda} \| p(\cdot, t) \|_{L^2(\Omega)} \kappa(t) = \gamma. \]
Herewith one obtains, cf. [24],
\[ \bar{u} = -\frac{1}{\lambda} p \cdot \min \left\{ 1, \frac{\gamma}{\| p(\cdot, t) \|_{L^2(\Omega)}} \right\}. \]
In case of \( \lambda = 0 \) one obtains a bang-bang control. The optimal control \( \bar{u}(\cdot, t) \) must always have a constant \( L^2(\Omega) \)-norm with value \( \gamma \) for all \( t \in (0, t_f) \); cf. Fig. 6.

Finally, differentiating the Lagrangian with respect to \( t_f \)
\[ \frac{d}{dt_f} \mathcal{L}(y, p, u, t_f) = 1 + \int_{x=0}^{1} \left( p_t(x, t_f) y_t(x, t_f) - p_x(x, t_f) y_x(x, t_f) \right) \]
\[ + u(x, t_f) p(x, t_f) \, dx \]
\[ + \frac{\lambda}{2} \int_{x=0}^{1} u^2(x, t_f) \, dx \]
\[ \begin{split}
- \int_{x=0}^{1} y_{tt}(x, t_f) \left( p(x, t_f) - \tilde{\beta}(x) \right) \\
+ y_t(x, t_f) p_t(x, t_f) \, dx \\
+ y_x(1, t_f) p(1, t_f) - y_x(0, t_f) p(0, t_f) \\
+ y(0, t_f) p_L(t_f) + y(1, t_f) p_R(t_f) \\
+ \int_{x=0}^{1} y_t(x, t_f) \beta(x) \, dx
\end{split} \]
\[ = -q_L(t_f) \]
\[ = 0 \quad = 0 \quad = 0 \quad = 0 \]
\[ \int_{x=0}^{1} y_t(x, t_f) \beta(x) \, dx = -p_x(x, t_f) \]
yields, by another partial integration, the transversality condition to determine the terminal time \( t_f \):
\[ 1 + \frac{\lambda}{2} \int_{x=0}^{1} u^2(x, t_f) \, dx \]
\[ + \int_{x=0}^{1} \left( y_{xx}(x, t_f) + u(x, t_f) \right) p(x, t_f) \]
\[ - y_t(x, t_f) p_t(x, t_f) \, dx = 0. \]

Note that the complete derivation is formal only, since it would be hardly possible to carry through an analysis as in [24], in more general cases.

Figures 5–7 show some numerical results obtained via FDTO; the pure bang-bang control behaviour becomes apparent due to the small regularization parameter \( \lambda \).

**B. The non-regularized minimum damping optimal control problem for the wave equation**

In order to get singular subdomains we modify this problem by requiring an objective, which damps the system towards zero state and velocity being certainly of interest for practical applications (damping of oscillations):
\[ \min J(y, u) = \min \frac{1}{2} \int_{0}^{t_f} \int_{0}^{1} y^2 + y_t^2 \, dx \, dt \]
subject to
\[ y_{tt}(x, t) - y_{xx}(x, t) = u(x, t) \text{ in } \Omega \times (0, t_f), \]
\[ g(x, 0) = y_1(x) \text{ in } \Omega, \]
\[ y_t(0, t) = y_2(x) \text{ in } \Omega, \]
\[ y(0, t) = 0 \text{ in } [0, t_f], \]
\[ y(1, t) = 0 \text{ in } [0, t_f], \]
again with \( \Omega = (0, 1) \), but now with \( t_f \) fixed and sufficiently large. The set \( U_{\text{ad}} \) of admissible controls remains unchanged.

Similarly as in the previous section, the formal Lagrange technique yields the following adjoint equation
\[ -p_{tt} + p_{xx} = y_{tt} - y \text{ on } \Omega \times (0, t_f), \]
\[ p(x, t_f) = 0 \text{ and } p_t(x, t_f) = -y_t(x, t_f) \text{ on } \Omega, \]
\[ p(0, t) = p(1, t) = 0 \text{ in } [0, t_f], \]
and the variational inequality for the optimal control
\[ (p, u - \bar{u})_{L^2((0,1) \times (0, t_f))} \geq 0 \forall u \in U_{\text{ad}}. \]

Hence the optimal control \( \bar{u} \) can be bang-singular according to the control law (pointwise in time):
\[ \bar{u} = \begin{cases} -\gamma \frac{p}{\| p \|_{L^2(\Omega)}}, & \text{if } \| p \|_{L^2(\Omega)} > 0; \\ y - y_{xx}, & \text{if } \| p \|_{L^2(\Omega)} \equiv 0. \end{cases} \]

Numerical results for this problem are shown in Figs. 8–10. The coincidence with the control law becomes apparent as well as the discontinuous transition from the bang-bang to the singular subdomain.
IV. A POSTPROCESSING METHOD FOR SWITCHING TIME OPTIMIZATION IN PDE OPTIMAL CONTROL

In practical applications control devices mostly depend on time only. If models require a distributed control \( u \) it can often be split into a prescribed spatial distribution \( \beta(x) \) and the actual time-dependent control \( v(t) \). In view of this we modify the preceding example by a new set of admissible controls

\[
U_{\text{ad}} := \{ u \in L^2(\Omega \times (0, t_f)) : u(x, t) = \beta(x) v(t) \text{ with } \beta \in L^2(\Omega) \text{ prescribed and } v \in L^2(0, t_f) \text{ with } v_a \leq v \leq v_b \text{ a.e. in } [0, t_f] \}
\]

with given \( L^\infty(0, t_f) \)-bounds \( v_a \) and \( v_b \). Hence the optimal control \( \bar{u} \) can also be bang-singular (pointwise in time):

\[
\bar{u} = \begin{cases} 
\beta v_a, & \text{if } \int_{\Omega} \beta p > 0, \\
\gamma - \beta y_{xx}, & \text{if } \int_{\Omega} \beta p \equiv 0, \\
\beta v_b, & \text{if } \int_{\Omega} \beta p < 0.
\end{cases}
\]

As in the previous example switches occur only along lines of constant time.

Figure 11 shows the optimal control resulting from a postprocessing switching point optimization, which relies only on information from primal variables: We start with a guess for the switching structure obtained by a precomputed FDTO approximation. Then we reformulate our optimization
problem. Since the control is given by its bounds on bang-bang subarcs, it has no longer to be considered as optimization variable there. Consequently, optimization variables are just the switching times and the discretized singular control. Note that singular control laws always constitute feedback laws; i.e., they depend only on state variables. However, we may find dependencies on higher derivatives of the state variable in OC-PDE; compare the examples in Subsection II-B and III-B. To make use of these formulae instead of discretizing the control on singular subdomains, higher-order difference scheme for discretizing the state variables would be required to approximate their derivatives sufficiently accurate. This effort will usually not pay.

Data and results for the switching times are given in the figure caption of Fig. 11.

![Fig. 11. Control u. Data: $y(x,0) = \sin(\pi x)$, $y_1(x,0) = 0$, $t_f = 3$, $v_a = -2.4$, $v_b = 2.4$, $\beta(x) = \sin(\pi x)$. Results: $t_1 \approx 1.00021$, $t_2 \approx 2.01582$](image)

In general, the application of such a postprocessing step is much more involved in OC-PDE as its analog in OC-ODE, since the zero level sets of switching functions may generally be curves or manifolds in the space-time cylinder. Shape optimization techniques may then come into play to determine these level sets, resp. the bang-bang and singular subdomains.

Finally, it must be mentioned that the optimal control problem of Subsection III-B is a rare example where the bounds on the control depend on the adjoint state. This is caused by the unusual control constraint chosen in [24], which however allows some nice theoretical analysis. Here the adjoints have to be exploited additionally so that the presented switching point optimization would no longer be a direct method in the OC-ODE sense.

In summary: if switching curves are straight lines constant in time, the number of optimization variables can be considerably reduced. Shape optimization techniques can be avoided then. Singular controls are still to be discretized as before, if they depend on higher derivatives of state variables. Otherwise feedback laws can be used, too.

V. CONCLUSIONS AND FUTURE WORKS

A. Conclusions

Optimal control problems for partial differential equations with bang-bang and singular controls have not found much interest so far since these problems resist a rigorous analytical treatment, although most of the problems originally show distributed or boundary controls appearing linearly, which is a prerequisite for the appearance of singular subdomains. The formal Lagrange technique seems to be the only way to develop candidates for necessary conditions because of non-linearities and the difficulty, if not impossibility, of an a priori detection of singular subdomains. Hence First-Discretize-Then-Optimize techniques provide the method of choice. The paper shows how the results can nevertheless be verified according to the optimal control law from theory, at least to a certain extent. A postprocessing method, similar to the switching time optimization technique for ODE constrained optimal control problems, can be applied in cases where the zero level sets of switching functions are straight lines. Herewith the numerical results can be improved, in particular the determination of the switching times, even with fewer optimization variables.

B. Future Works

Open problems are concerned with proofs of non-existence of singular subdomains, with singular subdomains in cases of boundary controls, and with the application of shape optimization techniques if zero level sets of switching functions are curves or manifolds in the space-time cylinder.

Shape optimization may be not only applicable in post-processing steps to improve numerical results for the primal variables from FDTO approaches but also to exploit the full set of necessary conditions of primal and dual variables similar to a new approach for state-constrained OC-PDE developed by Frey [17]. In his thesis, Frey has generalized the well-known Bryson-Denham-Dreyfus approach [4] for state-constrained OC-ODE to OC-PDE. He has reformulated state-constrained elliptic PDE optimal control problems as set optimal control problems by partitioning the domain $\Omega$ into sets where the state constraint is active, resp. inactive. Appropriate matching conditions then determine the interface between active and inactive sets. For its computation, Newton-like methods have been developed which are based on shape calculus, resp. optimization on vector bundles.

To transfer these ideas to the determination of subdomains where controls are bang-bang, resp. singular in the general case of zero level sets of switching functions being curves or manifolds would constitute an enormous analytical and numerical challenge. This approach would lead to an analogon to the multipoint boundary value problem formulation in ODE optimal control; cf., e.g., [6].

In addition, open problems refer to the connection of the order of a singular subdomain and the appearance of chattering controls. In this paper, the singular subdomains are all of first order, when we adopt the terminology of OC-ODE — here we have to apply one second order differential...
operator to the vanishing switching function to bring the singular control to light. Note that chattering controls have already been observed for OC-PDE in Theihßen’s thesis [37].

REFERENCES


