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This article is a preprint. It was published in Control and Cybernetics by the System Research Institute of the Polish Academy of Sciences. The version of record is available at http://control.ibspan.waw.pl:3000/contents/export?filename=2010-3-04_pesch_et_al.pdf.

On some new phenomena in state-constrained optimal control if ODEs as well as PDEs are involved

by

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Abstract: In this paper we investigate a new class of optimal control problems with ODE as well as PDE constraints. We would like to call them "hypersonic rocket car problems", since they were inspired, on the one hand, by the well known rocket car problem from the early days of ODE optimal control, on the other hand by a recently investigated flight path trajectory optimization problem for a hypersonic aircraft.

The hypersonic rocket car problems mimic the latter's coupling structure, yet in an strongly simplified form. They can therefore be seen as prototypes of ODE-PDE control problems. Due to their relative simplicity they allow to a certain degree to obtain analytical solutions and insights into the structure of the adjoints, which would currently be unthinkable with complex real life problems.

Our main aim is to derive and verify necessary optimality conditions. Most of the obtained results bear a lot of similarities with state constrained ODE optimal control problems, yet we also observed some new phenomena.

Keywords: Optimal control of partial differential equations, ODE-PDE-constrained optimization, state constraints, non-local state-constraints, integro-state constraints, optimal control problems for integro-differential equations, jump conditions.

1. Introduction

Realistic mathematical models for applications with a scientific or engineering background often have to consider different physical phenomena and therefore may lead to coupled systems of equations that include partial and ordinary differential equations. While each of the fields of optimal control of partial resp. ordinary differential equations has already been subject to thorough research, the optimal control of systems containing both has not been studied widely in literature, neither theoretically nor numerically.

One of the few examples was an optimal control problem recently studied by M. Wächter (2004) and Chudej et. al. (2009). It describes the flight of a hypersonic aircraft under the objective of minimum fuel consumption. The flight trajectory is described, as usual, by a system of ordinary differential equations (ODE). This system is controlled by the usual control variables of flight path optimization under various control and state variable inequality constraints. However, due to the hypersonic flight conditions a thermal protection system is indispensable and must therefore be taken into account in the model. Therefore the ODE system has to be augmented by a quasi-linear heat equation with non-linear boundary conditions. It is coupled with the ODEs through its boundary conditions. A major goal of the optimization is the limitation of the heating of the thermal protection system. This leads to a pointwise state constraint for its temperature. This constraint couples the PDE with the ODE reversely. However the enormous complexity of this problem only allowed numerical analysis.

In the present paper we will consider a model problem as simple as possible while still including the key features of this real-life ODE-PDE optimal control problem. Thereby we hope to achieve some insight into the structure of those problems and their solutions.

We would like to call that simplified model problem the "hypersonic rocket car problem". To one part it consists of the classical "rocket car on a rail track problem" from the early days of ODE control, first studied by Bushaw (1952). Fel'dbaum (1949) has studied similar problems of that type even earlier. He particularly focussed the attention to the importance of optimal processes of linear systems for automatic control. The behaviour of their optimal controls was later called bang-bang. The second part is a one dimensional heat equation with a source term depending on the speed of the car, denoting the heating due to friction.

Other variants of hypersonic rocket car problems will be investigated in Pesch et. al. (in preparation).

2. The hypersonic rocket car problem

In the following, the ODE state variable w denotes the one-dimensional position of the car depending on time t with the terminal time t_f unspecified. The PDE state variable T stands for the temperature and depends on time as well as

the spatial coordinate x describing the position within the car. The control u denotes the acceleration of the car. The PDE is controlled only indirectly via the velocity \dot{w} of the car like a distributed control. Obviously, boundary control problems can also be formulated and will be published subsequently (Pesch et. al., in preparation).

The aim is to drive the car in minimal time from a given starting position and speed (w_0 resp. \dot{w}_0) to the origin of the phase plane while keeping its temperature below a certain threshold T_{\max} .

All in all, the hypersonic rocket car problem considered here is given as follows:

$$\min_{u \in U} \left\{ t_f + \frac{1}{2} \lambda \int_0^{t_f} u^2 dt \right\}, \quad \lambda > 0, \quad (1a)$$

subject to

$$\ddot{w}(t) = u(t) \quad \text{in } (0, t_f), \quad (1b)$$

$$w(0) = w_0, \quad \dot{w}(0) = \dot{w}_0, \quad (1c)$$

$$w(t_f) = 0, \quad \dot{w}(t_f) = 0, \quad (1d)$$

$$U := \{u \in L^2(0, t_f) : |u(t)| \leq u_{\max} \text{ almost everywhere in } [0, t_f]\}, \quad (1e)$$

and

$$\frac{\partial T}{\partial t}(x, t) - \frac{\partial^2 T}{\partial x^2}(x, t) = \dot{w}(t)^2 \text{ in } (0, 1) \times (0, t_f), \quad (1f)$$

$$T(x, 0) = T_0 \text{ on } (0, 1), \quad (1g)$$

$$-\frac{\partial T}{\partial x}(0, t) = -(T(0, t) - T_0), \quad \frac{\partial T}{\partial x}(1, t) = -(T(1, t) - T_0) \text{ on } [0, t_f], \quad (1h)$$

and finally subject to a pointwise state constraint of type

$$T(x, t) \leq T_{\max} \text{ almost everywhere in } (0, 1) \times (0, t_f). \quad (1i)$$

The initial temperature T_0 of the car is in the following set to zero. In the numerical experiments the regularisation parameter λ is chosen as $\frac{1}{10}$ and the control constraint u_{\max} as 1.

3. The state-unconstrained problem and its associated temperature profile

For better illustration and to alleviate comparison with the numerical results of section 5.1. let us first have a brief look at the solution of the state unconstrained (i. e. only ODE) problem:

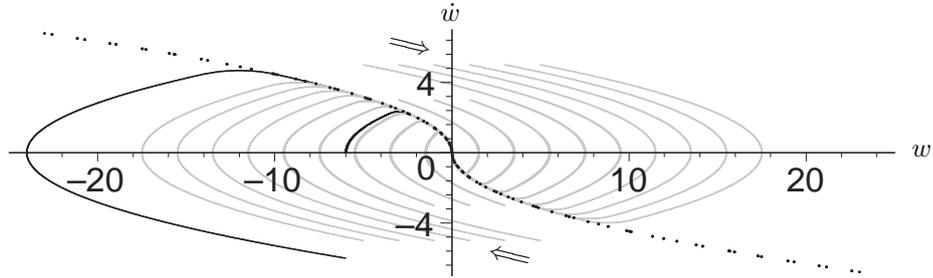


Figure 1. Optimal trajectories of the regularized minimum-time problem in the phase plane (grey). The dotted black curve is their envelope curve. The black curves are the optimal solutions for the starting conditions $w_0 = -6$ and $\dot{w}_0 = 0$ resp. $w_0 = -6$ and $\dot{w}_0 = -6$. Those will be picked up again later on.

Furthermore, the heat equation itself can be solved analytically, which will be very helpful for later analysis:

$$\begin{aligned} T(x, t) &= \sum_{n=1}^{\infty} \left[\int_0^t \dot{w}(s)^2 e^{-k_n^2 (t-s)} ds \right] \cdot \left(\int_0^1 \phi_n(y) dy \right) \phi_n(x) \\ &= \sum_{n=1}^{\infty} \left[\int_0^t \dot{w}(s)^2 e^{-k_n^2 (t-s)} ds \right] \cdot \frac{1}{N_n} \left[\sin k_n + \frac{1}{k_n} (1 - \cos k_n) \right] \phi_n(x) \quad (2) \end{aligned}$$

This solution is obtained by Fourier's method and some rather longsome computations, which are omitted here; see Pesch et. al. (in preparation).

The eigenvalues k_n are determined by

$$\frac{2k_n}{k_n^2 - 1} = \tan k_n \quad (3)$$

and the normed eigenfunctions by

$$\phi_n(x) = \frac{1}{N_n} (k_n \cos k_n x + \sin k_n x) \quad (4)$$

with the norming factor

$$N_n = \sqrt{\frac{1}{2}k_n^2 + \frac{3}{2}}. \quad (5)$$

Herewith one can compute the temperature profiles of the two trajectories shown in Fig. 1:

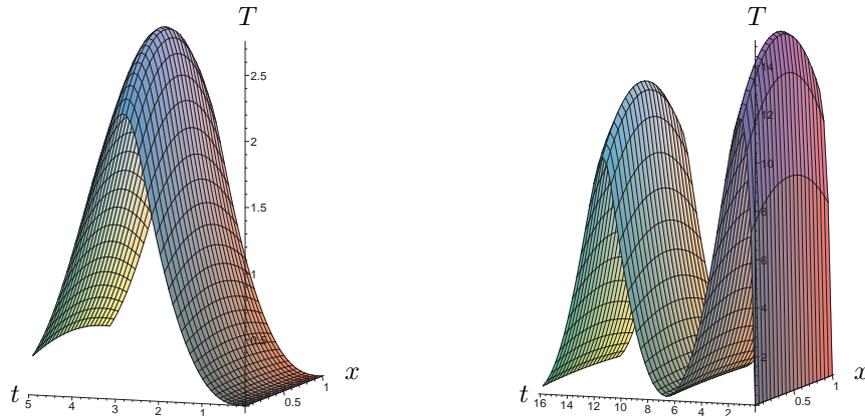


Figure 2. Temperature profiles along state-unconstrained trajectories; cf. Figure 1. Data: $w_0 = -6$, $\dot{w}_0 = 0$ (left), resp. $\dot{w}_0 = -6$ (right).

Please note that (1f) represents distributed heating, therefore the maximal temperature with respect to space is always reached at $x = \frac{1}{2}$; see below. Modelling the heating of the car's nose by a boundary control is done in Pesch et al. (in preparation).

The double hump structure of the heat profile for the $(w_0 = \dot{w}_0 = -6)$ -curve is due to the initial velocity pointing in the wrong direction, which makes it necessary to slow down and turn around first.

To round of this prelude we would like to present some useful properties of the solution T of the heat equation, namely that it is positive in $[0, 1] \times (0, t_f]$ and possesses strong maxima w.r.t. x for all $t > 0$ on the vertical line $x = \frac{1}{2}$ (as already stated above).

THEOREM 1 *Let $T(x, t)$ be a solution of (1b)-(1h) with the following properties:*

- (A1) T is continuous in $[0, 1] \times [0, t_f]$, $\partial_x^i T$, $i = 1, \dots, 3$, as well as $\partial_x^i T_t$, $i = 0, 1$, exist and are continuous in $[0, 1] \times (0, t_f]$;
- (A2) T_x possesses a continuation in $C^0([0, 1] \times [0, t_f])$, also denoted by T_x .

Then there holds:

- a) If $\dot{w}^2 > 0$ for $[0, 1] \times (0, t_f]$, then $T > 0$ in $[0, 1] \times (0, t_f]$.
- b) $T(x, t) = T(1 - x, t)$.
- c) T takes its strong maximum in $x = \frac{1}{2}$ for each $t_0 \in (0, t_f]$. $T(x, t_0)$ increases strictly monotonic in $[0, \frac{1}{2}]$ and decreases strictly monotonic in $[\frac{1}{2}, 1]$.

The proof of this theorem and further theorems concerning also other hypersonic-rocket-car problems can be found in Pesch et al. (in preparation).

4. Necessary optimality conditions: Interpretation as integro state-constrained ODE optimal control problem

Deriving necessary optimality conditions proved to be relatively challenging due to the problem being very nonstandard. Therefore we first had to reformulate it: The second order ODE (1) was transformed into a system of two first order ODEs with the new variables $w_1 := w$ and $w_2 := \dot{w}$. Additionally, one can utilize the fact, that at any given point of time the maximum of the temperature with respect to x is at $x = \frac{1}{2}$, by introducing an auxiliary state variable

$$w_3(t) := T\left(\frac{1}{2}, t; w_2[0, t]\right) = \int_0^t \sum_{n=1}^{\infty} \tilde{\gamma}_n w_2(s)^2 e^{-k_n^2(t-s)} ds \quad (6)$$

with

$$\tilde{\gamma}_n = \left(\int_0^1 \phi_n(y) dy\right) \phi_n\left(\frac{1}{2}\right) \quad \text{and} \quad \sum_{n=1}^{\infty} \tilde{\gamma}_n = 1. \quad (7)$$

Here it is important to notice, that T does not only depend on the current speed w_2 but on its entire history, due to the integral term in (6). This will play a crucial role later on.

The usual way to exploit necessary conditions by means of an adjoint based method, formerly called indirect method, is as follows; cp., e.g. Pesch (1994): Firstly, compute a numerical solution of the state unconstrained problem, to be more precise an approximation for a candidate optimal solution. One of the most powerful methods here is the multiple shooting method. See for example, Bulirsch (1971), Stoer, Bulirsch (2002), Oberle (1983) and for some approved codes, Oberle (1989), resp. Hiltmann et. al. (1993). The expected switching structure (hypothesis) can usually be guessed via homotopy methods by tightening the state constraint step by step.

Let us now assume, that exactly one boundary arc $(t_{\text{on}}, t_{\text{off}})$, $t_{\text{on}} < t_{\text{off}}$ exists. (This will be the case for $w_0 = -6$, $\dot{w}_0 = 0$). The reformulated problem is then given as:

$$\min_{u \in U} \left\{ t_f + \frac{1}{2} \lambda \int_0^{t_f} u^2 dt \right\}, \quad \lambda > 0, \quad (8a)$$

subject to

$$\dot{w}_1(t) = w_2(t) \quad \text{in } (0, t_f), \quad (8b)$$

$$\dot{w}_2(t) = u(t) \quad \text{in } (0, t_f), \quad (8c)$$

$$\dot{w}_3(t) = \frac{d}{dt} T\left(\frac{1}{2}, t; w_2[0, t]\right) \quad \text{in } (0, t_f), \quad (8d)$$

$$w_1(0) = w_0, \quad w_2(0) = \dot{w}_0, \quad (8e)$$

$$w_1(t_f) = 0, \quad w_2(t_f) = 0, \quad (8f)$$

$$w_3(t_{\text{on}}) = T_{\text{max}} \quad \text{and} \quad w_3(t_{\text{off}}) = T_{\text{max}}, \quad (8g)$$

$$w_3(0) = 0, \quad (8h)$$

$$w_3(t) - T_{\text{max}} \leq 0 \quad \text{in} \quad (0, t_f), \quad (8i)$$

$$U := \{u \in L^2(0, t_f) : |u(t)| \leq u_{\text{max}} \text{ almost everywhere in } [0, t_f]\}, \quad (8j)$$

We were able to get completely rid of the PDE part and now have a pure ODE problem. This of course comes at a high price: equation (8d) is a Volterra integro-differential equation, making this new problem significantly more complicated than a standard ODE optimal control problem. Only little is known on optimal control problems with integro-differential equations; see Kappel, Stettner (1976), Schmidt (2001), or Warga (1972). At least, the new state constraint (8i) is pointwise and of second order (see below), whereas (1i) with T substituted by (2) constitutes a non-local state constraint.

Defining $S(t, \mathbf{w}, T) := T\left(\frac{1}{2}, t\right) - T_{\text{max}}$ with $\mathbf{w} := (w_1, w_2, w_3)^T$ two (total) differentiations w. r. t. t yield ($[t]$ shall in the following be an abbreviaton of the list of all arguments evaluated at time t that apply to the respective function)

$$\frac{d}{dt}S[t] = T_t\left(\frac{1}{2}, t\right) = T_{xx}\left(\frac{1}{2}, t\right) + w_2(t)^2, \quad (9a)$$

$$\frac{d^2}{dt^2}S[t] = T_{tt}\left(\frac{1}{2}, t\right) = T_{xxt}\left(\frac{1}{2}, t\right) + 2w_2(t)u(t). \quad (9b)$$

Here, both the ODE (8c) and the PDE (1f) are substituted.

The junction points t_{on} and t_{off} are implicitly defined by (8g). They will give rise to jump conditions.

In order to derive the adjoint equations for (8), we apply the Lagrange technique, for the sake of simplicity, formally only; see, e.g. Tröltzsch (2009).

Let the Lagrangian be defined by

$$\begin{aligned} \mathcal{L}(\mathbf{w}, u, \mathbf{p}, t_{\text{on}}, t_{\text{off}}, t_f) := & \int_0^{t_f} 1 + \frac{\lambda}{2} u^2 dt - \int_0^{t_f} (\dot{w}_1 - w_2) p_1 dt \\ & - \int_0^{t_f} (\dot{w}_2 - u) p_2 dt \\ & - \int_0^{t_f} \left[\dot{w}_3 - \frac{d}{dt}T\left(\frac{1}{2}, t; w_2[0, t]\right) \right] p_3 dt \\ & + \int_0^{t_f} (w_3 - T_{\text{max}}) d\mu(t) \end{aligned}$$

$$+(w_3(t_{\text{on}}) - T_{\text{max}}) \sigma_{\text{on}} + (w_3(t_{\text{off}}) - T_{\text{max}}) \sigma_{\text{off}} .$$

Integration by parts then yields, while substituting (1d) and (8h),

$$\begin{aligned} \mathcal{L}(\mathbf{w}, u, \mathbf{p}, t_{\text{off}}, t_f) &:= \int_0^{t_f} 1 + \frac{\lambda}{2} u^2 \, dt + [w_1 p_1]_{t=0} + \int_0^{t_f} w_1 \dot{p}_1 + w_2 p_1 \, dt \\ &\quad + [w_2 p_2]_{t=0} + \int_0^{t_f} w_2 \dot{p}_2 + u p_2 \, dt \\ &\quad - [w_3 p_3]_{t=t_f} + \int_0^{t_f} w_3 \dot{p}_3 + \frac{d}{dt} T \left(\frac{1}{2}, t; w_2[0, t] \right) p_3 \, dt \\ &\quad + \int_0^{t_f} (w_3 - T_{\text{max}}) \mu(t) \, dt \\ &\quad + (w_3(t_{\text{on}}) - T_{\text{max}}) \sigma_{\text{on}} + (w_3(t_{\text{off}}) - T_{\text{max}}) \sigma_{\text{off}} . \end{aligned}$$

Here, we give the derivation of the adjoint p_2 only:

$$\begin{aligned} D_{w_2} \mathcal{L}(\dots) h_2 &= \int_0^{t_f} p_1(t) h_2(t) \, dt + \int_0^{t_f} \dot{p}_2(t) h_2(t) \, dt \\ &\quad + \int_0^{t_f} 2 w_2(t) h_2(t) p_3(t) \, dt \\ &\quad - \int_0^{t_f} \left(\int_0^t \sum_{n=1}^{\infty} k_n^2 \tilde{\gamma}_n 2 w_2(s) e^{-k_n^2 (t-s)} h_2(s) \, ds \right) p_3(t) \, dt \\ &\stackrel{\text{Fubini}}{\implies} \int_0^{t_f} p_1(t) h_2(t) \, dt + \int_0^{t_f} \dot{p}_2(t) h_2(t) \, dt \\ &\quad + \int_0^{t_f} \left(2 w_2(t) p_3(t) \right. \\ &\quad \left. - \int_t^{t_f} \sum_{n=1}^{\infty} k_n^2 \tilde{\gamma}_n 2 w_2(t) e^{-k_n^2 (s-t)} p_3(s) \, ds \right) h_2(t) \, dt \stackrel{!}{=} 0 \end{aligned}$$

for all $h_2 \in W^{1,\infty}(0, t_f)$ with $h_2(0) = 0$.

This yields

$$\dot{p}_2 = -p_1 - 2 w_2(t) \left(p_3(t) - \int_t^{t_f} \sum_{n=1}^{\infty} k_n^2 \tilde{\gamma}_n e^{-k_n^2 (s-t)} p_3(s) \, ds \right), \quad (10a)$$

a retrograde integro-differential equation of Volterra type.

All other necessary conditions turn out the way they would in a classical ODE control problem:

$$\dot{p}_1 = 0, \quad (10b)$$

$$\dot{p}_3 = -\mu$$

$$\text{and } p_3(t_f) = 0 \quad \text{and } p_3(t_{\text{on/off}}^+) = p_3(t_{\text{on/off}}^-) - \sigma_{\text{on/off}}$$

$$\text{with } \sigma_{\text{on/off}} > 0, \quad (10c)$$

$$H[t_f] = 0, \quad H[t_{\text{on/off}}^+] = H[t_{\text{on/off}}^-] \quad (10d)$$

$$\begin{aligned} \text{with } H(\mathbf{w}, u, \mathbf{p}) := & 1 + \frac{\lambda}{2} u^2 + w_2 p_1 + u p_2 \\ & + \frac{d}{dt} T\left(\frac{1}{2}, t; w_2[0, t]\right) p_3 \end{aligned} \quad (10e)$$

$$u(t) = P_{[-u_{\max}, u_{\max}]} \left(-\frac{1}{\lambda} p_2 \right) \quad (10f)$$

$$\text{with } P_{[a,b]}(z) := \min \{b, \max \{a, z\}\},$$

$$\mu = \begin{cases} 0 & \text{on } [0, t_{\text{on}}] \cup (t_{\text{off}}, t_f] \\ \geq 0 & \text{on } [t_{\text{on}}, t_{\text{off}}] \end{cases} \quad \text{and } \mu(w_3 - T_{\max}) = 0. \quad (10g)$$

REMARK 1 *As constraint (8i) is of second order, there can appear not only boundary arcs but also touch points, cf. Figure 8. Necessary conditions for this scenario can be derived analogously, the interior point condition*

$$T\left(\frac{1}{2}, t_{\text{touch}}; w_2[0, t_{\text{touch}}]\right) = T_{\max}$$

will cause a jump of p_3 at t_{touch} .

5. Numerical results

5.1. Solution of the state-constrained problem

Solving the seemingly relatively simple (original) problem (1) already invokes a level of complexity which makes, at the current state of the art, an indirect "first optimize, then discretize"- approach a vain or at least extremely cumbersome endeavour, leaving the direct "first discretize, then optimize"-method as the more promising technique. For numerical calculations we employed the interior point

solver IPOPT (2007) by A. Wächter and Biegler (2002), resp. (2006) together with the modelling software AMPL (2007). The use of AMLP guarantees that all gradients are efficiently computed by automatic differentiation.

The first step was a time transformation $\tau := \frac{t}{t_f}$ to a normalized time $\tau \in [0, 1]$, resulting in a problem with fixed terminal time at the cost of spawning an additional optimization variable t_f . Applying a quadrature formula to (1a), discretizing the ODE with the implicit midpoint rule and the PDE with the Crank-Nicolson scheme yielded a nonlinear program which could then be solved by IPOPT. The results are shown in Figures 3 and 4:

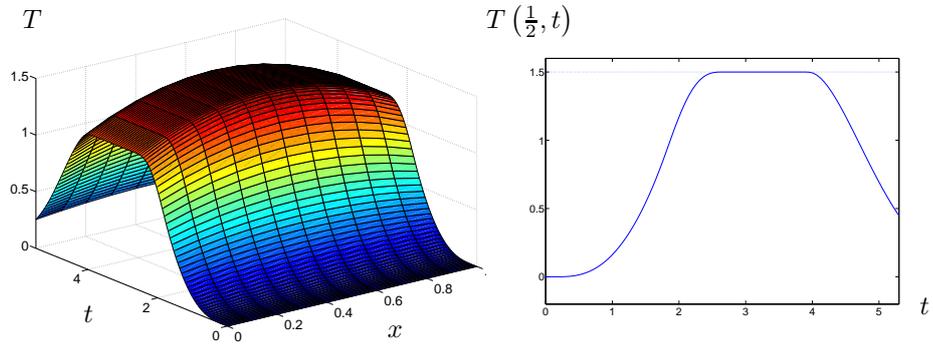


Figure 3. Temperature $T(x, t)$ (left) and cross-section $T(\frac{1}{2}, t)$ (right) along a state-constrained trajectory. Data: $w_0 = -6$, $\dot{w}_0 = 0$ and $T_{\max} = 1.5$, cf. Figures 1 and 2 (left).

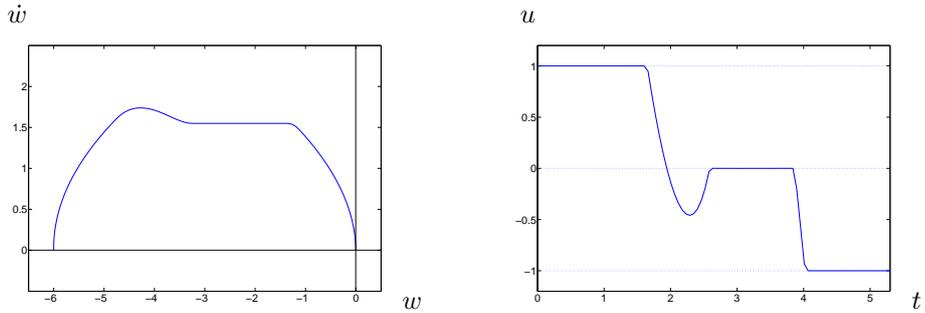


Figure 4. State-constrained optimal trajectory in the phase-plane (left) with associated optimal control u (right). Data: $w_0 = -6$, $\dot{w}_0 = 0$ and $T_{\max} = 1.5$.

Figure 3 depicts the temperature profile as well as its cross-section at $x = \frac{1}{2}$, clearly showing the boundary subarc. In Figure 4 one can see the according speed and position in the phase diagram and the optimal control.

Please note that the optimal control u is very small yet not identically zero between t_{on} and t_{off} as could be the impression from the picture. The most unusual feature is the nonlinear behaviour of the control immediately before t_{on} , which is also responsible for the little hump in the phase diagram. This is caused by a "memory effect" introduced by the heat equation (resp. by the lag property of (8d) in the alternative formulation). To our knowledge, this phenomenon has not yet been observed in ODE optimal control theory.

5.2. Verification of the necessary conditions

The main interest is of course not just to solve the problem, but to verify the necessary conditions, represented by the multipoint boundary value problem (10). To our knowledge, no off-the-shelf software seems to be available for problems like that. Therefore we verified (10) by using the discrete approximations of the adjoints for (8) obtained from IPOPT.¹

Figures 5–7 provide some visualization for the more complex equations:

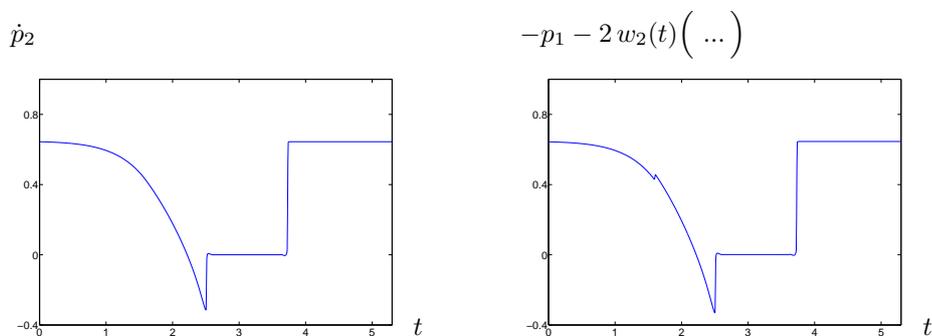


Figure 5. Left- and right-hand side of (10a)

¹Note that IPOPT delivers estimates for the adjoint variables with opposite sign compared to our notation.

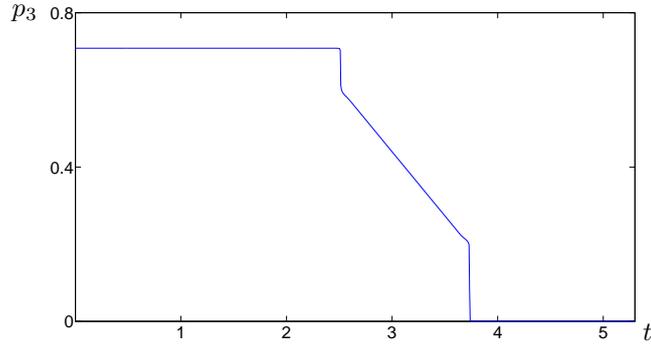


Figure 6. Estimated ODE adjoint p_3 with jumps $\sigma > 0$ and complementarity condition $\mu > 0$, conf. (10c)

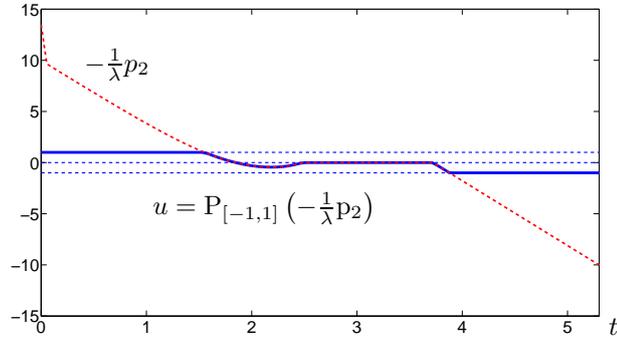


Figure 7. Optimality check showing the perfect coincidence with the projection formula (10f)

Furthermore $p_1 = \text{const} \approx 0.6$ and $H[t_f] = 0$. The inequality constraints (8i) and (8j) are also perfectly observed. Continuity of the Hamiltonian at the junction points follows immediately from the continuity of the optimal control.

As already mentioned in Remark 1, touch points are possible, too. Their necessary conditions can be derived analogously, so as a conclusion of the numerics we would just like to give a glimpse at the according results; see Fig. 8.

For more details on this we refer to Pesch et. al. (in preparation).

6. Conclusions and outlook

The problem studied in this paper has been inspired by problems from engineering control applications, where complex dynamical processes are described by staggered systems of equations of different type such as ODEs and PDEs. It can

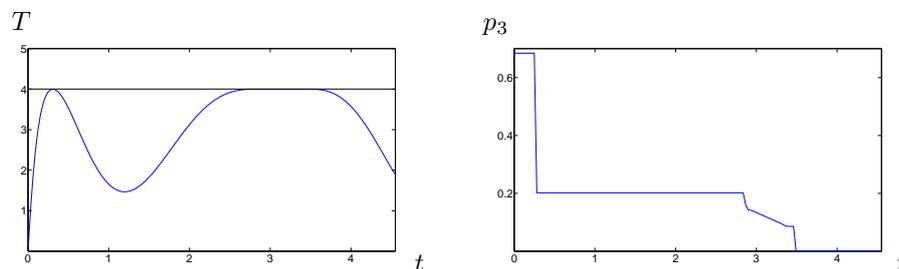


Figure 8. Temperature and adjoint p_3 for the case $w_0 = -6$ and $\dot{w}_0 = -6$ (cf. Figure 1 and Remark 1), clearly showing a touch point and the according jump in the adjoint. Here, T_{\max} has been changed to 4 and $u_{\max} = \infty$, to prevent infeasibility.

be seen as a kind of prototype for ODE-PDE control systems. As it has been stripped of anything but the most necessary ingredients we were able to account for the approximate validity of the necessary conditions based on discrete estimates of the adjoint variables. At the current state of the art the application of an adjoint based method for such a problem remains a tremendous challenge.

In this paper we transformed the ODE-PDE control problem into an only ODE (yet nonstandard) problem. It is also possible to do it the other way round, resulting in an only PDE problem (of course also nonstandard), which is a splendid opportunity to carry over concepts from ODE to PDE optimal control. However, this would go beyond the scope of this short paper. Some first results can be found in Wendl et. al. (2010).

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