On a State-Constrained PDE Optimal Control Problem arising from ODE-PDE Optimal Control

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Summary. The subject of this paper is an optimal control problem with ODE as well as PDE constraints. As it was inspired, on the one hand, by a recently investigated flight path optimization problem of a hypersonic aircraft and, on the other hand, by the so called "rocket car on a rail track"-problem from the pioneering days of ODE optimal control, we would like to call it "hypersonic rocket car problem". While it features essentially the same ODE-PDE coupling structure as the aircraft problem, the rocket car problem's level of complexity is significantly reduced. Due to this fact it is possible to obtain more easily interpretable results such as an insight into the structure of the active set and the regularity of the adjoints. Therefore, the rocket car problem can be seen as a prototype of an ODE-PDE optimal control problem. The main objective of this paper is the derivation of first order necessary optimality conditions.

Key words: Optimal control of partial differential equations, ODE-PDE-constrained optimization, state constraints

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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 theoretically so far to the best knowledge of the authors.
Recently Chudej et. al. [5] and M. Wächter [12] studied an optimal control problem numerically which describes the flight of an aircraft at hypersonic speed under the objective of minimum fuel consumption. The flight trajectory is described, as usual, by a system of ordinary differential equations (ODE). Due to the hypersonic flight conditions aerothermal heating of the aircraft must be taken into account. This leads to a quasi-linear heat equation with non-linear boundary conditions which is coupled with the ODE. As it is the main objective of the optimization to limit the heating of the thermal protection system, one obtains a pointwise state constraint, which couples the PDE with the ODE reversely. However, anything beyond mere numerical analysis is prohibited by the considerable complexity of this problem. Therefore the present paper's focus is a model problem stripped of all unnecessary content while still including the key features of ODE-PDE optimal control, which will allow a clearer view on the structure of the problem and its solution.
This simplified model problem we would like to call 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 [3]. 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.
In contrast to [10], which deals with the same ODE-PDE problem but from the ODE point of view, this paper is dedicated to a PDE optimal control approach.
Another even more complicated optimal control problem for partial integro-differential-algebraic equations including also ODEs, which describes the dynamical behaviour of the gas flows, the electro-chemical reactions, and the potential fields inside a certain type of fuel cells, has been investigated in [6], also numerically only. However, this model does not include a state constraint.

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.

The aim is to drive the car in minimal time from a given starting position and speed (w_0 resp. v_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 is given as follows:

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

subject to

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

$$w(0) = w_0\,, \quad \dot{w}(0) = v_0\,, \tag{1c}$$

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

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

and

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

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

$$-\frac{\partial T}{\partial x}(0,t) = -\big(T(0,t) - T_0(0)\big)\,,$$

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

and finally subject to a pointwise state constraint of type

$$T(x,t) \le T_{\max} \text{ in } [0,l]\times[0,t_f]\,. \tag{1i}$$

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 $\frac{1}{10}$, the length l of the car and the control constraint $u_{\max}$ both as 1, and the source term $g(\dot{w}(t))$ as $\dot{w}(t)^2$, which models the temperature induced by friction according to Stokes' law (proportional to the square of the velocity).

3 The state-unconstrained problem and its associated temperature profile

For better illustration and to alleviate comparison with the numerical results of section 5 let us first have a brief look at the solution of the state unconstrained (i. e. only ODE) problem; see Fig. 1. This figure describes the optimal solutions for all starting values in the w-$\dot{w}$-phase plane converging into the origin. Unlike the non-regularized problem ($\lambda = 0$) with a pure bang-bang switching structure and optimal solutions having at most one switching point when its trajectories cross the switching curve (dotted black), on which the car finally arrives at the origin, the optimal solutions of the regularized problem ($\lambda > 0$) have a transition phase between two bang-bang subarcs. The smaller the regularization parameter λ is the closer the optimal trajectories (grey) approach the switching curve which serves as their envelope here.

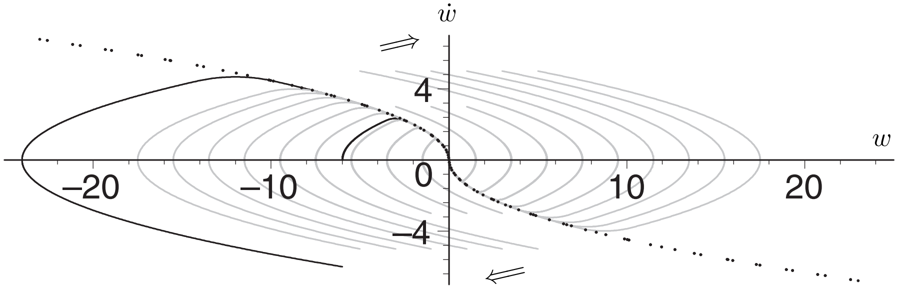

Fig. 1. Optimal trajectories of the regularized minimum-time problem ($\lambda > 0$) in the phase plane (grey). The dotted black curve is the switching curve of the non-regularized problem ($\lambda = 0$). The black curves are the optimal solutions for the starting conditions $w_0 = -6$ and $v_0 = 0$ resp. $w_0 = -6$ and $v_0 = -6$.

Along those two trajectories the following temperature profiles emerge:

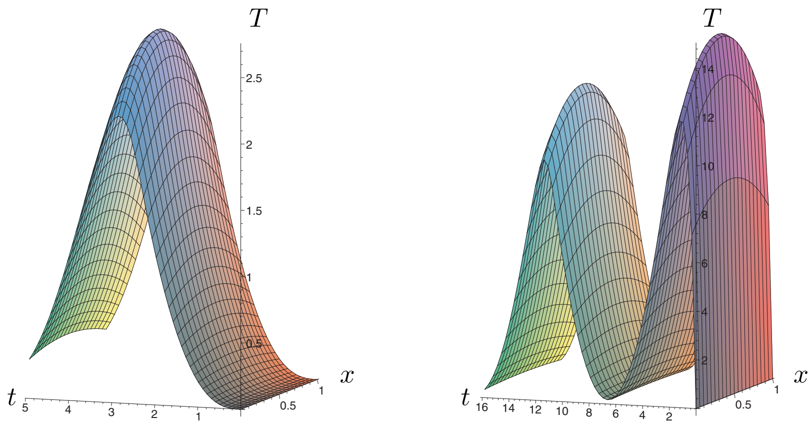

Fig. 2. Temperature profiles along the state-unconstrained trajectories due to the data $w_0 = -6$, $v_0 = 0$ (left), resp. $v_0 = -6$ (right); see Fig. 1.

Those temperature profiles have to be bounded in the following; cp. Fig. 3.

4 Necessary optimality conditions: Interpretation as state-constrained PDE optimal control problem

It is possible to reformulate (1) as a PDE optimal control problem by eliminating the ODE-part:

$$\int_0^{t_f} \left(1 + \frac{\lambda}{2}\, u^2(t)\right) \,\mathrm{d}t \stackrel{!}{=} \min_{|u| \le u_{\max}} \tag{2a}$$

subject to

$$T_t(x,t) - T_{xx}(x,t) = \left(v_0 + \int_0^t u(s)\,\mathrm{d}s\right)^2 \quad \text{in } (0,l) \times (0,t_f)\,, \tag{2b}$$

$$-T_x(0,t) + T(0,t) = 0\,, \quad T_x(l,t) + T(l,t) = 0 \quad \text{for } 0 < t < t_f\,, \tag{2c}$$

$$T(x,0) = 0 \quad \text{for } 0 \le x \le l\,, \tag{2d}$$

$$\int_0^{t_f} u(t)\,\mathrm{d}t = -v_0\,, \tag{2e}$$

$$\int_0^{t_f} \int_0^t u(s)\,\mathrm{d}s\,\mathrm{d}t = -w_0 - v_0\,t_f \stackrel{\text{part. int.}}{\Longrightarrow} \int_0^{t_f} t\,u(t)\,\mathrm{d}t = w_0\,, \tag{2f}$$

$$T(x,t) \le T_{\max} \quad \text{in } [0,l] \times [0,t_f]\,. \tag{2g}$$

Here the term $v(t) := v_0 + \int_0^t u(s)\,\mathrm{d}s$ plays the role of a "felt" control for the heat equation. The two isoperimetric conditions (2e, f) are caused by the two terminal conditions (1c) and comprehend the constraints (1b–d) of the ODE part. While this reformulation will alleviate the derivation of first order necessary conditions,it nevertheless comes at a price, namely the nonstandard structure of (2e, f) and especially the source term in (2b). All these terms contain the control under integral signs.

The existence and uniqueness of the solution $T \in W_2^{1,0}((0,l) \times (0,t_f)) \cap C([0,t_f], L^2(0,l))$, the Fréchet-differentiability of the solution operator and the existence of a Lagrange multiplier $\bar{\mu} \in C([0,l] \times [0,t_f])^* = \mathcal{M}([0,l] \times [0,t_f])$ [the set of regular Borel measures on $([0,l] \times [0,t_f])$] under the assumption of a local Slater condition are proven in [8], [9]. Moreover, it turns out, that T is of even higher regularity: T_{tt} and $\partial_x^4 T$ are both of class $L^r(\varepsilon, t_f; L^2(0,l))$ with $0 < \varepsilon < t_f$ and $r \ge 2$ for all controls $u \in L^2(0,t_f)$.

Thereby, we can establish the optimality conditions by means of the Lagrange technique. Furthermore it can be seen that for any given point of time [and for every control $u \in L^2(0,t_f)$] the maximum of T with respect to space is obtained right in the middle at $x = \frac{l}{2}$ (cf. Fig. 2; for a proof see [8]). This implies, that the active set $\mathcal{A}$ is a subset of the line $L := \{x = \frac{l}{2},\ 0 < t < t_f\}$.

Hence the state constraint can equivalently be replaced by $T \leq T_{\max}$ on L. Using this we define the Lagrange-function by

$$\begin{aligned}\mathcal{L} = &\int_0^{t_f} \left(1 + \frac{\lambda}{2}\, u^2(t)\right)\,\mathrm{d}t - \int_0^{t_f}\!\!\int_0^l \Big(T_t - T_{xx} - g\big(v_0 + \textstyle\int_0^t u(s)\,\mathrm{d}s\big)\Big)\, q\,\mathrm{d}x\,\mathrm{d}t \\ &- \int_0^{t_f} \big(-T_x(0,t) + T(0,t)\big)\, q(0,t)\,\mathrm{d}t - \int_0^{t_f} \big(T_x(l,t) + T(l,t)\big)\, q(l,t)\,\mathrm{d}t \\ &+ \nu_1 \left(\int_0^{t_f} u(t)\,\mathrm{d}t + v_0\right) + \nu_2 \left(\int_0^{t_f} t\, u(t)\,\mathrm{d}t - w_0\right) \\ &+ \int_0^{t_f} \left(T(\frac{l}{2}, t) - T_{\max}\right) \mathrm{d}\mu(t)\,, \end{aligned} \tag{3}$$

with $\mu(t) \in \mathcal{M}(0, t_f)$ and the multipliers q associated with the constraints (2b–c) respectively $\nu_1\,, \nu_2 \in \mathbb{R}$ associated with (2e, f).

By partial integration and differentiation of (3) we find the necessary conditions of first order ($*$ shall in the following denote optimal values):

Adjoint equation:

$$\begin{aligned}&\int_0^{t_f^*}\!\!\int_0^l q_t\, \psi - q_x \psi_x\,\mathrm{d}x\,\mathrm{d}t - \int_0^{t_f^*} q(0,t)\, \psi(0,t)\,\mathrm{d}t - \int_0^{t_f^*} q(l,t)\, \psi(l,t)\,\mathrm{d}t \\ &\quad + \int_0^{t_f} \psi(\frac{l}{2}, t)\,\mathrm{d}\mu(t) = 0 \quad \text{for all } \psi \in W(0, t_f^*)\,, \end{aligned} \tag{4a}$$

$$q(x, t_f^*) = 0 \quad \text{for almost all } x \in [0, l]\,, \tag{4b}$$

Variational inequality:

$$\begin{aligned}&\int_0^{t_f^*} \big(\lambda u^*(t) + \nu_1 + \nu_2\, t\big)\, \big(u(t) - u^*(t)\big)\,\mathrm{d}t \\ &+ \int_0^{t_f^*} g'\big(v_0 + \textstyle\int_0^t u^*(r)\,\mathrm{d}r\big) \left(\displaystyle\int_0^t u(s) - u^*(s)\,\mathrm{d}s\right) \left(\int_0^l q(x,t)\,\mathrm{d}x\right) \mathrm{d}t \geq 0 \\ &\overset{\text{Fubini}}{\Longrightarrow} \int_0^{t_f^*} \left[\lambda u^*(t) + \nu_1 + \nu_2\, t + \int_t^{t_f^*} g'\big(v_0 + \textstyle\int_0^s u^*(r)\,\mathrm{d}r\big) \left(\displaystyle\int_0^l q(x,s)\,\mathrm{d}x\right) \mathrm{d}s\right] \cdot \\ &\qquad \big(u(t) - u^*(t)\big)\,\mathrm{d}t \geq 0\,, \quad \text{for all } u \in U\,, \end{aligned} \tag{4c}$$

Complementarity condition:

$$\mu \geq 0\,, \quad \int_0^{t_f^*} \left(T^*(\frac{l}{2}, t) - T_{\max}\right) \mathrm{d}\mu(t) = 0\,. \tag{4d}$$

The optimality system is completed by a condition for the free terminal time t_f^* and two conditions that give the switching times t_{on}^*, t_{off}^* [i. e. the times where the temperature $T^*(\frac{l}{2}, t)$ hits, resp. leaves the constraint $T_{\max}$, cf. Fig. 3 (right)]. As the derivation of these condition would exceed the scope of this paper they will be published in subsequent papers [8] and [9].

Equations (4a, b) represent the weak formulation of the adjoint equation, which is retrograde in time, and can be formally understood as

$$-q_t(x,t) - q_{xx}(x,t) = \mu(t)\,\delta(x - \frac{l}{2}) \text{ in } (0,l) \times (0,t_f^*)\,, \tag{5a}$$

$$-q_x(0,t) = -q(0,t)\,,\ q_x(l,t) = -q(l,t) \text{ on } [0,t_f^*] \quad \text{and}$$

$$q(x,t_f^*) = 0 \text{ on } [0,l]\,. \tag{5b}$$

Since the adjoints can be interpreted as shadow prices, the line $\{\frac{l}{2}\} \times (t_{\mathrm{on}}^*, t_{\mathrm{off}}^*)$ indicates from where the temperature exerts an influence on the objective functional. This result corresponds to the structure of the solution of the initial-boundary value problem to be expected from (4a, b), in particular $q(x,t) \equiv 0$ for $t_{\mathrm{off}}^* \le t \le t_f^*$; cf. Fig. 5.

A key condition is the optimality condition (4c) which determines the optimal control. It is a complicated integro-variational inequality with a kernel depending on all values of u^* on the interval $[0, t_f^*]$, forward in time, as well as on all values of q on $[t, t_f^*]$, backward in time. Instead (4c), we can determine the optimal control by an integro-projection formula,

$$u^*(t) = P_{[-u_{\max}, u_{\max}]}\left\{ -\frac{1}{\lambda} \left[\nu_1 + \nu_2\, t + \int_t^{t_f^*} g'(v^*(s)) \left(\int_0^l q(x,s)\,\mathrm{d}x \right) \mathrm{d}s \right] \right\}. \tag{6}$$

Comparing this result with the analogous projection formula of [10] it turns out that the second factor [in squared brackets] is just the adjoint velocity $p_{\dot{w}}(t)$ of the equivalent ODE optimal control formulation with the PDE eliminated analytically by a Fourier-type series. This formulation however is also of non-standard form (with a non-local state constraint leading to boundary value problems for systems of complicated integro-ODEs); see [10].

5 Numerical results

The numerical calculations were conducted with the interior point solver IPOPT [7], [11] by A. Wächter and Biegler in combination with the modelling software AMPL [1], with the latter featuring automatic differentiation. This first-discretize-then-optimize (direct) approach was chosen, because even the ostensibly simple and handsome problem (1) proves to be a "redoubtable opponent" for a first-optimize-then-discretize (indirect) method.

After a time transformation $\tau := \frac{t}{t_f}$ to a problem with fixed terminal time (at the cost of spawning an additional optimization variable t_f), applying a simple quadrature formula[1] to (1a), discretizing the ODE with the implicit midpoint rule and the PDE with the Crank-Nicolson scheme, one obtains a nonlinear program to be solved with IPOPT.

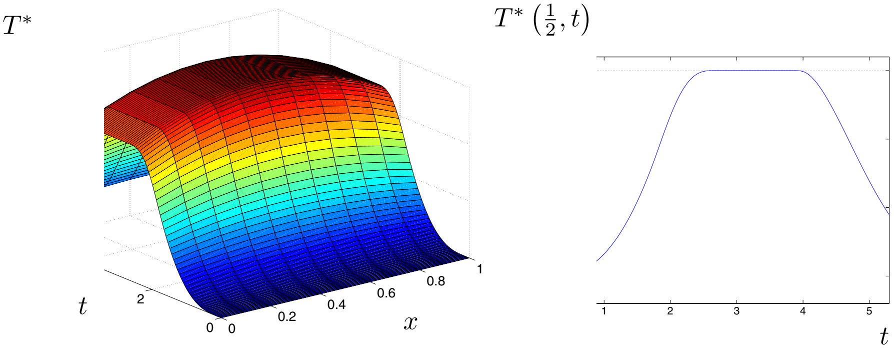

Fig. 3. Temperature $T^*(x,t)$ (left) and cross-section $T^*\left(\frac{1}{2},t\right)$ (right) along the state-constrained trajectory due to the data $w_0 = -6$, $v_0 = 0$, and $T_{\max} = 1.5$, cf. Figs. 1 and 2 (left).

The approximation of the optimal temperature is shown in Fig. 3. The set of the active state constraint, the line segment $\mathcal{A} = \{\frac{l}{2}\} \times [t^*_{\text{on}}, t^*_{\text{off}}]$, can clearly be seen. The computations used a space-time discretization of 100 by 1000 grid points yielding $t^*_f = 5.35596$, overall objective functional value of 5.51994, $t^*_{\text{on}} = 2.53$ and $t^*_{\text{off}} = 3.96$.

Figure 4 shows the approximations of the optimal control (solid) and the adjoint velocity $p_{\dot{w}}$ (dashed) from the ODE optimal control problem investigated in [10] and also obtained by IPOPT.[2] The perfect coincidence with the projection formula (6) becomes apparent; note the remark to (6).

Figure 5 depicts the approximation of the discrete adjoint temperature yielded by IPOPT[2]. With a closer look at q one can observe a jump discontinuity of its derivative in spatial direction along the relative interior of $\mathcal{A}$. This corresponds to the known jump conditions for adjoints on interior line segments in state-constrained elliptic optimal control [2]. Furthermore one can notice two Dirac measures as parts of the multiplier μ at the entry and exit points of $\mathcal{A}$ in analogy to the behaviour of isolated active points [4]. On the

[1] a linear combination of the trapezoidal sum and the trapezoidal rule with equal weights 1 which indeed approximates a multiple of the integral (2a), but avoids any oscillations of the control.

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

other hand the multiplier μ contains a smooth part in the relative interior of $\mathcal{A}$ reminiscent of the common behaviour in ODE optimal control.

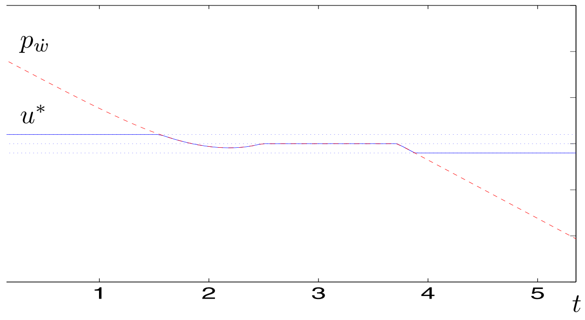

Fig. 4. Optimality check according to the projection formula (6)

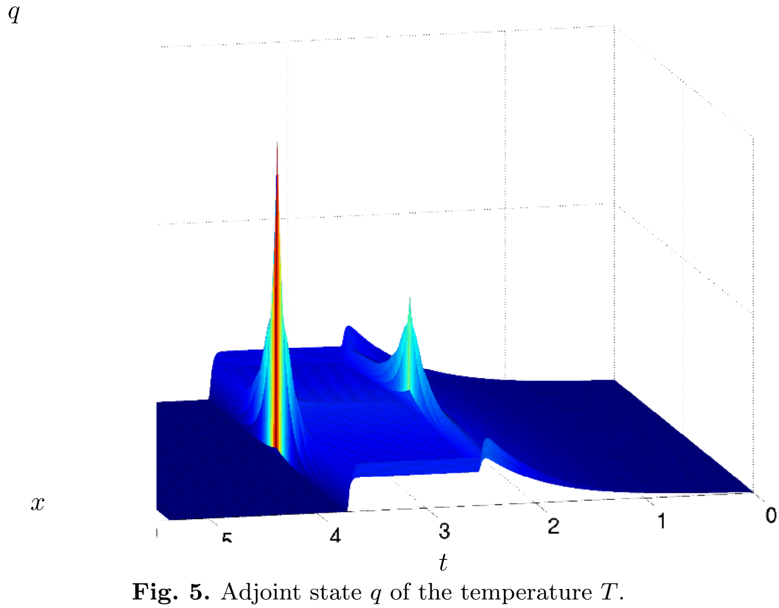

Fig. 5. Adjoint state q of the temperature T.

6 Conclusion

In this paper we studied a prototype of an ODE-PDE optimal control problem. As it is of relatively simple structure, it allows an unobstructed view on its adjoints and optimality system. However an adjoint based method even for such a seemingly simple model problem still remains a formidable task, leaving a direct method as a much more convenient way to go. This of course results in the downside that one has to content oneself with estimates of the continuous

problems' adjoints obtained from the discrete adjoints of the NLP solver used in the *first-discretize-then-optimize* approach.
Transforming the ODE-PDE problem into an only PDE problem, as it has been done in this paper is not the only possibility of tackling it. As it is also viable to transform it into an only ODE problem, which will of course also be pretty nonstandard, an interesting opportunity to compare concepts of ODE and PDE optimal control may arise here such as statements on the topology of active sets. However this is beyond the limited scope of the present paper but can be found in [8], [9].

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