Transformation approach to constraint handling in optimal control of the heat equation

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Abstract: In this contribution, an approach is presented for the optimal control of the boundary-controlled heat equation, which is subject to state- and input-constraints. Thereby, suitably chosen asymptotic saturation functions are used to reformulate the original infinite-dimensional system in new coordinates. The new unconstrained optimal control problem can then be solved with methods of unconstrained optimization. The method is demonstrated for a heat-up problem where both state and input constraints become active.

Keywords: Constrained control; optimal control; control of heat transfer systems; control of partial differential equations

1. INTRODUCTION

Optimal control of infinite-dimensional systems described mathematically by partial differential equations (PDEs) is a field in control theory, which at the same time is well established and has sparked new interest in more recent years, in part due to the increase in computing power (see, e.g., Lions, 1970; Fattorini, 1999; Hinze et al., 2009). Possible applications arise in nearly every physical domain if very accurate mathematical models are called for.

One of the basic equations for the theory of PDE control is the heat equation, which also often arises in applications. A principal control task is the heating up (or cooling down) of a certain workpiece as rapidly as possible. Thereby it is often essential to respect certain constraints concerning both the actuators as well as the workpiece temperature itself in order to avoid damaging either one. Since the handling of constraints is difficult to include in most classical control design methods, optimization-based approaches are an appropriate choice (Eppler and Tröltzsch, 2001; Steinboeck et al., 2011).

The numerical solution of constrained optimal control problems (OCPs) – both if the underlying system dynamics is infinite-dimensional or finite-dimensional – usually follows either a direct approach by discretizing the OCP in order to obtain a finite-dimensional constrained optimization problem (Bock and Plitt, 1984; Hargraves and Paris, 1987; Agrawal and Faiz, 1998; Betts, 1998) or alternatively by using an indirect approach, where the classical optimality conditions are solved numerically (Bryson and Ho, 1969; Pesch, 1994; Bonnans and Hermant, 2009). In particular in the literature on optimal control for systems governed by partial differential equations, also the notions of first discretize then optimize and first optimize then discretize are used, respectively (Hinze et al., 2009). In either case, the solution of the constrained OCP typically requires considerable numerical effort, which makes it, for instance, difficult to use in online applications like receding horizon control, although dedicated algorithms are available nowadays (Diehl et al., 2002; Zavala and Biegler, 2009; Houska et al., 2011).

One method to relax this problem consists in transforming the constrained OCP into an unconstrained one and finally to use efficient numerical methods of unconstrained (dynamic) optimization to solve the optimal control problem. This approach was primarily developed for finite-dimensional systems described mathematically by ordinary differential equations in Graichen and Petit (2009); Graichen et al. (2010), and has already allowed for computational efficiency improvements, in particular in online applications (Käpernick and Graichen, 2013).

In this contribution, the approach as it is presented in Graichen et al. (2010); Graichen and Petit (2009) is transferred to the heat equation as a prototype for parabolic PDEs. It is demonstrated how the OCP for a heat-up process is transformed from constrained to unconstrained coordinates. The resulting unconstrained OCP is then solved with an optimization method using full discretization. Motivated by the results of Käpernick and Graichen (2013), the presented method is particularly promising as a novel approach to online optimization and model predictive control of systems governed by PDEs.

The paper is structured as follows: In Section 2, the mathematical model of the heat-up problem is defined and the transformation to unconstrained coordinates is carried out. In Section 3, the OCP is formulated both in constrained and in unconstrained coordinates, and the relation of the two formulations is discussed. After some remarks concerning the numerical solution of the optimal control problem in Section 4, simulation results are shown in Section 5, before the paper is concluded by a short summary and outlook in Section 6.
2. PROBLEM STATEMENT

In this contribution, the boundary-controlled heat equation on a one-dimensional spatial domain \( z \in [0, 1] \) is considered, which is given as

\[
\begin{align*}
\partial_t x - q \partial_x^2 x &= 0 \quad (1a) \\
\partial_x x \big|_{z=0} &= 0, \quad (1b) \\
q_0 \partial_x x \big|_{z=1} &= u - q_1 x \big|_{z=1} \quad (1c)
\end{align*}
\]

with the state \( x := x(t, z) \), the boundary control input \( u := u(t) \), the strictly positive constant parameters \( q \), \( q_0 \), and \( q_1 \), and suitable initial conditions \( x(0, z) = x_0(z) \).

This system is subject to state and control input constraints of the form

\[
x \in [x^-, x^+] \quad \text{and} \quad u \in [u^-, u^+] \quad (2)
\]

whereby symmetry with respect to 0 is assumed for simplicity, i.e., \( x^- = -x^+ \) and \( u^- = -u^+ \).

2.1 Saturation functions

In order to remove the explicitly formulated state and control input constraints from the problem formulation, asymptotic saturation functions are used as a state transformation. For this, a system variable \( a \) with constraints \( a^\pm \) is replaced by

\[
a = \psi(a, a^\pm) \quad (3)
\]

where \( a \) is the new, unconstrained system variable. Besides guaranteeing that \( a \) is within its constraints, the saturation functions are required to satisfy the following conditions

- The transformation has to be sufficiently smooth and strictly monotonically increasing, i.e.,
  \[
  \partial_a \psi(a, a^\pm) > 0 \quad (4)
  \]
- The saturation functions have to be asymptotic in the sense that \( \psi(a, a^\pm) \to a^\pm \) for \( a \to \pm \infty \).
- The second-order derivative in the first argument may be expressed in terms of the first-order derivative with respect to the first argument, i.e.,
  \[
  \partial_a^2 \psi(a, a^\pm) = d(a) \partial_a \psi(a, a^\pm) \quad (5)
  \]

whereby it is guaranteed that \( d(a) \) remains bounded for all \( a \). Note that this property can be extended to higher-order derivatives, which, however, is not necessary in the problem considered in this work.

A suitable choice of the saturation function is

\[
\psi(a, a^\pm) = a^+ - \frac{a^+ - a^-}{1 + \exp \left( \frac{4a}{a^+ - a^-} \right)} \quad (6)
\]

as shown in Figure 1. In this case, \( d(a) \) is given as

\[
d(a) = -\frac{4(\exp(4a/(a^+ - a^-)) - 1)}{(a^+ - a^-)(1 + \exp(4a/(a^+ - a^-)))},
\]

which can be easily confirmed to be bounded for all \( a \). The saturation function furthermore designed to be scaled in such a way that \( \partial_a \psi(a, a^\pm) \big|_{a=0} = 1 \), which is beneficial for the numerical experiments shown in the further course of this contribution.

1 Except at the place of definition, arguments are dropped for brevity of notation.

Fig. 1. Asymptotic saturation function (6) with saturation bounds \( a^\pm \).

2.2 Transformation to unconstrained coordinates

In order to apply the transformation by means of saturation functions to the system (1), first a saturation function (3) is used to substitute the state variable, i.e., \( x = \psi(\xi, x^+) \) with the new state \( \xi := \xi(t, z) \). Using this substitution in all the derivatives of as they appear in (1) and using the property (5) yields

\[
\begin{align*}
\partial_\xi x &= \partial_\xi \psi(\xi, x^+) \partial_\xi \xi \\
\partial_\xi x &= \partial_\xi \psi(\xi, x^+) \partial_\xi \xi \\
\partial_\xi x &= \partial_\xi \psi(\xi, x^+) (\partial_\xi \xi)^2 + \partial_\xi \psi(\xi, x^+) \partial_\xi^2 \xi \\
&= \partial_\xi \psi(\xi, x^+) \left[ d(\xi)(\partial_\xi \xi)^2 + \partial_\xi^2 \xi \right] \quad (7c)
\end{align*}
\]

Subsequently, the infinite-dimensional system (1) may be rewritten in the new unconstrained state \( \xi \). Using the property (4) the PDE (1a) can be written as

\[
\partial_\xi^2 \psi(\xi, x^+) \left[ \partial_\xi \xi - q \left( \partial_\xi^2 \xi + d(\xi)(\partial_\xi \xi)^2 \right) \right] = 0 \\
\quad \Leftrightarrow \quad \partial_\xi \xi - q \left( \partial_\xi^2 \xi + d(\xi)(\partial_\xi \xi)^2 \right) = 0 \quad (8a)
\]

and by analogous considerations, the boundary condition (1b) becomes

\[
\partial_\xi \xi \big|_{z=0} = 0 \quad (8b)
\]

Concerning the boundary condition (1c), additional considerations have to be carried out. Applying the transformation (3) to the state \( x \big|_{z=1} \) and solving for \( \partial_\xi \xi \big|_{z=1} \) yields

\[
\partial_\xi \xi \big|_{z=1} = \frac{u - q_1 \psi(\xi \big|_{z=1}, x^\pm)}{q_0 \partial_\xi \psi(\xi \big|_{z=1}, x^\pm)} \quad (9)
\]

Since \( u \) is known to be constrained, it is an obvious choice to replace the right hand side of (9) by another saturation function. The bounds of this saturation function are determined as

\[
\frac{u^+ - q_1 \psi(\xi \big|_{z=1}, x^\pm)}{q_0 \partial_\xi \psi(\xi \big|_{z=1}, x^\pm)} \leq \partial_\xi \xi \big|_{z=1} \leq \frac{u^+ - q_1 \psi(\xi \big|_{z=1}, x^\pm)}{q_0 \partial_\xi \psi(\xi \big|_{z=1}, x^\pm)} \quad (10)
\]

and as opposed to the bounds of the state variable are not constant but depend on the boundary state \( \xi \big|_{z=1} \). Thus, the boundary condition for \( z = 1 \) of the new, unconstrained system can be given as

\[
\partial_\xi \xi \big|_{z=1} = \psi(v, \phi^\pm(\xi \big|_{z=1})) \quad (11)
\]

where \( v := v(t) \) is introduced as the new and unconstrained control input. The control input of the constrained system (1) in terms of the unconstrained coordinates \( \xi \) and \( v \) can be determined using (9) and (11) as
\[ u = q_0 \partial_\xi \psi(\xi|z=1, x^\pm) \psi(v, \phi^\pm(\xi|z=1)) + q_1 \psi(\xi|z=1, x^\pm) =: \chi(v, \xi|z=1), \quad (12) \]
such that in summary, a transformation
\[ x = \psi(\xi, x^\pm) \]
\[ u = \chi(v, \xi|z=1) \]
is obtained, which is bijective between the state \( x \) and the input \( u \) from the open intervals defined by the respective constraints and the unbounded coordinates \( \xi \) and \( v \).

3. CONstrained AND UNconstrained OPTIMAL CONTROL

The optimal control task to be carried out for the finite-dimensional system (1) is the heat-up from an initial state profile \( x_0 \) to a desired state profile \( x^* \).

3.1 Formulation of the OCP

This control task may be formulated as an OCP as follows
\[
\text{OCP}_x: \quad \min_u \int_0^T l(x, u) dt \\
\text{s.t.} \quad \begin{cases}
\partial_t x = q_0 \partial_\xi^2 x \\
\partial_\xi x|_{z=0} = 0 , \\
q_0 \partial_\xi x|_{z=1} = u - q_1 x|_{z=1} , \\
x \in [x^-, x^+], \quad u \in [u^-, u^+].
\end{cases} \quad (14)
\]

Thereby, the running cost \( l(x, u) \) of the optimization problem is chosen as a standard quadratic cost penalizing the deviation from the desired stationary state \( x^* \) and control input \( u^* \), i.e.,
\[
l(x, u) = \frac{1}{2} \|x - x^*\|^2_Q + \frac{r}{2}(u - u^*)^2 \quad (15)
\]
where \( \|\cdot\|^2_Q \) denotes the weighted \( L^2 \)-norm with the weight \( Q(z) = 10 \) (no dependence on the spatial coordinate is considered here) for the state and the weight \( r = 1 \) for the control input.

In the transformed and thus unconstrained coordinates, the OCP \( (14) \) is noted as follows
\[
\text{OCP}_\xi: \quad \min_v \int_0^T l(\xi, v) + p(v) dt \\
\text{s.t.} \quad \begin{cases}
\partial_\xi \xi = q \left( \partial_\xi^2 \xi + d(\xi) (\partial_\xi \xi)^2 \right) \\
\partial_\xi \xi|_{z=0} = 0 \\
\partial_\xi \xi|_{z=1} = \psi(v, \phi^h(\xi|z=1))
\end{cases} \quad (16)
\]

Thereby, the running cost is at first the transformation of (15) to the coordinates of the unconstrained problem
\[
l(\xi, v) = \frac{1}{2} \|\psi(\xi, x^\pm) - x^*\|^2_Q + \frac{r}{2}(\chi(v, \xi|z=1) - u^*)^2 . \quad (17)
\]
but is amended with an additional penalty
\[
p(v) = \frac{\epsilon}{2} v^2 \quad (18)
\]
with the (potentially small) constant parameter \( \epsilon > 0 \). This penalty can be understood as a regularization term weighting the new control input \( v \), which is necessary to account for the fact that the state and input transformation (13) is only defined on the open intervals of the constraints. \( ^2 \) An interpretation of the penalty term (18) is given in terms of the constrained variables \( x \) and \( u \) in the next Section 3.2 as well as in terms of the (discretized) optimality conditions in Section 4.2.

3.2 Interpretation of the additional penalty \( p(v) \)

In order to show the influence of the penalty (18), OCP \( \xi \) in (16) can be transformed back into the original variables \( x \) and \( u \) via the inverse transformation in (13). This leads to the following OCP \( \xi \) with the original dynamics and the penalized cost of the form
\[
\text{OCP}_\xi: \quad \min_u \int_0^T l(x, u) + \tilde{p}(x, u) dt \\
\text{s.t.} \quad \begin{cases}
\partial_t x = q_0 \partial_\xi^2 x \\
\partial_\xi x|_{z=0} = 0 , \\
q_0 \partial_\xi x|_{z=1} = u - q_1 x|_{z=1} .
\end{cases}
\]

where \( \tilde{p}(x, u) = p(\chi^{-1}(u, x|z=1)) \) is evaluated for \( v = \chi^{-1}(u, x|z=1) \) and using \( \xi|_{z=1} = \psi^{-1}(x|z=1, x^\pm) \) from the transformation (13). In detail, \( \tilde{p}(x, u) \) becomes
\[
\tilde{p}(x, u) = \frac{\epsilon}{2} \left[ \ln \frac{u - u^-}{u^+ - u} \right] \left( \frac{(u^+ - u^-)(x^+ - x^-)^2}{16q_0(x|z=1 - x)(x^+ - x|z=1)} \right)^2 . \quad (20)
\]

It is obvious from the structure of (20) that \( \tilde{p}(x, u) \) becomes unbounded as soon as \( x|z=1 \) or \( u \) approach their respective bounds except for \( u = (u^+ + u^-)/2 \). Hence, the inclusion of (18) in the OCP \( \xi \) corresponds to an interior barrier function that replaces the original constraints of OCP \( x \) in (14).

Two aspects of this result remain to be discussed: firstly, the fact that the barrier function does not come into effect in the particular case \( \tilde{p}(x, (u^+ + u^-)/2) = 0 \), and secondly, that only the state evaluated at the controlled boundary \( x|z=1 \) is considered by the use of (18). These issues can be resolved by taking into account some of the properties of the linear heat equation (1a). According to the maximum principle (see, e.g., Friedman, 1964; Widder, 1975), the state \( x \) assumes its maximum value at the controlled boundary. Thus, by assuring \( x^- < x|z=1 < x^+ \) it is guaranteed that the same applies for the complete state \( x(t, z) \). By similar considerations and by taking into account the symmetry of the state and input constraints with respect to \( 0 \) as well as the boundary condition (1c), it is clear that the state constraints \( x^\pm \) cannot be violated for \( u = 0 \).

4. NUMerical IMPLEMENTATION

In the following lines, a first discretize then optimize-approach is pursued to solve OCP \( \xi \), which necessitates a suitable semi-discretization of the infinite-dimensional system in (16).
4.1 Semi-discretization

For the spatial discretization, the so-called method of lines-approach is used with finite differences (see, e.g., Schiesser, 1991; Thomas, 1995). For this, the spatial coordinate $z$ is partitioned in a possibly non-equidistant grid with the nodes $z_i$, $i = 1, \ldots, N$, and element lengths $h_i = z_{i+1} - z_i$, $i = 1, \ldots, N - 1$. The semi-discretization of the unconstrained infinite-dimensional system (8a), (8b), and (11) then is formulated using central differences with some standard approximations concerning the discretization of the boundary conditions (8b) and (11) as

$\dot{z}_i = \frac{2q}{h_i^2}(\xi_i - \xi_{i+1}) + \frac{q}{h_i}d(\xi_i)(\xi_{i+1} - \xi_{i-1})$ \hspace{1cm} (21a)

$\dot{\xi}_i = \frac{2q}{h_i + h_{i-1}} \left[ \frac{\xi_{i+1} - \xi_i}{h_i} - \frac{\xi_i - \xi_{i-1}}{h_{i-1}} \right] + q d(\xi_i) \xi_{i+1} - \xi_i - h_{i-1}$, \hspace{1cm} $i = 2, \ldots, N - 1$ \hspace{1cm} (21b)

$\dot{\xi}_{N-1} = \frac{2q}{h_{N-1}}(h_{N-1}N^{-}(\psi(\xi_{i+1}) + \xi_{N-1} - \xi_N)$

\hspace{1cm} $- \frac{q d(\xi_N)}{h_{N-1}}(\xi_N - \xi_{N-1}) \times (2h_{N-1}-\psi(\xi_{i+1}) + \xi_{N-1} - \xi_N)$ \hspace{1cm} (21c)

which is noted briefly as $\dot{\xi} = f(\xi, v)$ and where the state variables represent the evaluation of the infinite-dimensional state $\xi$ at the grid nodes $z_i$, i.e., $\xi = [\xi_1 = \xi_{i=z=z_1}, \ldots, \xi_N = \xi_{i=z=z_N}]^T$.

The number of nodes $N$ is determined in the following accordingly to the respective needs in terms of precision.

The choice of finite differences as a means of discretization is by no means the only one possible, see, e.g., Hinze et al. (2009) and the references therein. However, it is rather simple in application and sufficient for the precision required in the subsequently shown simulation examples.

The discretized version of the OCP $\phi_1$ (16) can be noted as

$$\text{OCP}_{\phi_1} : \min_{\xi} \int_0^T \tilde{l}(\xi, v) + p(v) dt$$

subject to $\dot{\xi} = f(\xi, v)$, $\xi(0) = \xi_0$

with the discretized running cost (17) according to $\tilde{l}(\xi, v) = \frac{1}{2}\psi(\xi, x^\pm) - x^* \tilde{Q}\psi(\xi, x^\pm) - x^*$

$$+ \frac{r}{2} (\chi(v, x_N) - u^*)^2$$ \hspace{1cm} (23)

Thereby, the desired state is given in discretized form as $x^* = [x_1 = x_{i=z=z_1}, \ldots, x_N = x_{i=z=z_N}]^T$.

and the weight of the state variable $\tilde{Q} = \text{diag}(\tilde{Q}_i)$ has to be chosen in order to account for the spatial discretization.

4.2 Regularization of the finite-dimensional OCP

In the finite-dimensional setting, a further justification can be given for the inclusion of the penalty (18) considering the first-order optimality conditions. For this, the Hamiltonian of the OCP $\phi_1$ is defined as

$$H(\xi, v) = \tilde{l}(\xi, v) + \lambda^T f(\xi, v)$$ \hspace{1cm} (24)

with the adjoint state $\lambda = [\lambda_1, \ldots, \lambda_N]^T$. For the time being, it is assumed that $\psi(\xi, x^\pm) = v$, i.e., no constraint is imposed on the control input. One component of the first-order optimality conditions is the vanishing partial derivative of the Hamiltonian with respect to the control input $v$, i.e.,

$$\partial_v l(\xi, v) = \partial_v \tilde{l}(\xi, v) + \lambda^T \partial_v f(\xi, v) + cv = 0$$ \hspace{1cm} (25)

The respective components can be easily determined from (21) and (23) as

$$\partial_v \tilde{l}(\xi, v) = r_1(\chi(v, \xi_N) - v^*) \partial_v \lambda(v, \xi_N)$$ \hspace{1cm} (26)

and

$$\lambda^T \partial_v f(\xi, v) = 2q \lambda_N (1 + d(\xi_N))(\xi_N - \xi_{N-1})$$ \hspace{1cm} (27)

Similar considerations to the one leading to (20) show that $\partial_v \chi(v, \xi_N)$ vanishes as soon as the state constraints $x^\pm$ are approached. Thus, the regularization term $cv$ in (25) is necessary to avoid singular arc effects and to maintain solvability of (25) with respect to $v$. The analogous computations become more involved for the additional consideration of control input constraints and are therefore not developed here.

5. SIMULATION RESULTS

In this section, various simulation results are presented for the transformation approach to constraint handling in optimal control as it was outlined in the previous sections. Thereby, the system parameters are chosen as $q = 2$, $q_0 = 0.5$, $q_1 = 1$, $x^\pm = \pm 1.2$, and $u^\pm = \pm 2$. The initial condition $x_0(z) = 0$ is the stationary profile for $u = 0$ and the desired profile is imposed by the stationary control input $u^* = 1$ as $x^*(z) = 1$. The length of the optimization horizon is chosen $T = 1$.

In all plots of the constrained system (1), the evaluation of the state trajectory $x$ at $z = z = [0, 0.25, 0.5, 0.75, 1]$ is shown. Note thereby, that no distinction is made in the notation between the infinite-dimensional states $x(t, z)$, $\xi(t, z)$ and their finite-dimensional counterparts $x(t), \xi(t)$, which can be realized by suitable interpolation and the choice of a sufficiently fine grid. Furthermore to test the quality of the optimization results, all obtained control inputs are applied to a semi-discretization of the original infinite-dimensional system (1) with $N^\text{sim} = 101$ nodes, and the resulting trajectories $x^\text{sim}$ are plotted as light dotted lines for comparison.

As a reference, first the constrained OCP $\phi_1$ (14) is solved using full discretization and an interior point method (see, e.g., Noedel and Wright, 2006). In Figure 2 the resulting state $x$ as well as the control input $u$ are shown. It can be observed that both the control input as well as at least a part of the state touch the prescribed state and control input constraints.

Turning to simulation results due to the presented transformation approach, Figure 3 shows the state $\xi$ at $z = 0$ (dashed) and at $z = 1$ (solid) as well as the unconstrained control input $v$ for the solution of the OCP $\phi_1$ (16) for different weights $\epsilon$ of the penalty expression (18). While the trajectories of $\xi_{i=z=z}$, which in the solution of the constrained OCP $\phi_1$ (cf. Figure 2) do not approach the constraints, are nearly identical irrespective of $\epsilon$, the influence...
6. SUMMARY AND OUTLOOK

In this contribution, a state- and control-constrained OCP for the boundary-controlled heat equation is presented. Asymptotic saturation functions are used to obtain a formulation of the OCP in new, unconstrained variables. Amended with an additional penalty for the new unconstrained control input, this OCP is solved using full discretization. The resulting optimal control closely approaches the results obtained by directly applying methods of constrained optimization.

The primary benefit of the approach is expected to become visible if it is used in online applications as model predictive control, where methods of constrained optimization are rather impractical and where numerical inaccuracies are attenuated by the feedback control (Rhein et al., 2014). Furthermore, the property that constraints (2) are intrinsically satisfied by the transformed system becomes particularly interesting if the optimization problem is to be solved with a method that uses numerical integration such as, e.g., the gradient method (Käpernick and Graichen, 2013). This as well as the transfer of the approach to problems described by other types of PDEs is subject to future research.

REFERENCES


Fig. 4. State $x$ and control input $u$ according to the solution of the unconstrained OCP$_x^\epsilon$ (16) for $\epsilon = 5 \times 10^{-4}$ (left) and $\epsilon = 5 \times 10^{-6}$ (right) as well as boundary state $x_{|z=1}$ and control input $u$ according to the solution of the constrained OCP$_x$ (14) (dashed lines).


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