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Optimization with Partial Differential Equations

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Strategies for Time-Dependent PDE Control using an Integrated Modeling and Simulation Environment. Part Two: Problems with Inequality Constraints

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STRATEGIES FOR TIME-DEPENDENT PDE CONTROL USING AN INTEGRATED MODELING AND SIMULATION ENVIRONMENT. PART TWO: PROBLEMS WITH INEQUALITY CONSTRAINTS

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ABSTRACT. In the first part of this article, we have shown how time-dependent optimal control for partial differential equations can be realized in a modern high-level modeling and simulation package. In this second part we extend our approach to (state) constrained problems. “Pure” state constraints in a function space setting lead to non-regular Lagrange multipliers (if they exist), i.e. the Lagrange multipliers are in general Borel measures. This will be overcome by different regularization techniques.

To implement inequality constraints, active set methods and interior point methods (or barrier methods) are widely in use. We show how these techniques can be realized in the modeling and simulation package COMSOL MULTIPHYSICS.

In contrast to the first part, only the one-shot-approach based on space-time elements is considered. We implemented a projection method based on active sets as well as a barrier method and compare these methods by a specialized PDE optimization program, and a program that optimizes the discrete version of the given problem.

1. INTRODUCTION

In the paper [14] we show how time-dependent optimal control problems can be solved using the equation-based modeling and simulation environment COMSOL MULTIPHYSICS¹. In this paper we extend this approach to solve time-dependent optimal control problems subjected to pointwise state constraints.

Throughout this paper we consider optimal control problems of the form

$$(1) \quad \min j(y, u)$$

subject to

$$(2) \quad \begin{aligned} y_t - By &= u_Q && \text{in } Q \\ \vec{n} \cdot \nabla y + \alpha y &= u_\Sigma && \text{on } \Sigma \\ y(0) &= y_0 && \text{in } \Omega \end{aligned}$$

and to pointwise constraints $y_a \leq \beta y + \gamma u \leq y_b$ (box constraints) or $y_c \leq \beta y + \gamma u$ (unilateral constraints). The constraints may be given on the whole space-time domain Q or on the boundary Σ .

In contrast to elliptic PDEs, only for space-dimension $N = 1$ the control-to-state-operator S maps $L^2(Q)$ into $L^\infty(Q)$. For boundary controlled problems, we do not have such regularity. This lack of regularity demands an additional assumption on the optimal state: we demand that the optimal state y^* is a function in $L^\infty(Q)$.

Even now, caused by the fact that for “pure” state constraints the associated Lagrange multipliers are i.g. Borel measures, some regularization techniques are necessary. For constraints given on the same domain as the control we can use the well investigated Lavrentiev regularization, see e.g. the works [18] or [16]. In the case of boundary control and constraints given on the space-time domain the Lavrentiev regularization cannot be applied. Here, some different regularization concepts are developed, examples can be found in [19] and [15]. The structure and underlying theory of the optimal control problem should be kept in mind when considering appropriate discretization schemes. When applying standard FEM discretization as in COMSOL MULTIPHYSICS, measures should be avoided. We therefore mainly consider regularized problem formulations in our experiments.

In this paper, we investigate two possible methods to handle state constraints. First, we use the regularization suggested in [15] in the parabolic boundary controlled case and the classical Lavrentiev regularization as discussed in [11] in the case of distributed control. The optimality system can in this case via a projection formula be implemented by a min/max-function.

Key words and phrases. Optimal control, parabolic PDEs, inequality constraints, COMSOL MULTIPHYSICS.

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Second, we test some barrier methods to eliminate the pointwise state constraints. In [17], Schiela shows that some barrier methods do not need any additional regularization if their order is arbitrary high; i.e. in some sense, barrier methods are self-regularizing. Here, the integration of a path-following algorithm into COMSOL MULTIPHYSICS needs only minor changes in comparison to the solution of problems without inequality constraints, see [14] for the numerical treatment of such problems using COMSOL MULTIPHYSICS.

This paper is organized as follows: In Section 2 we specify the optimality conditions and quote some results concerning the existence and uniqueness of a minimizer for the given class of problems.

In the following two sections, we describe different methods to handle inequality constraints algorithmically.

In Section 4, we show how the optimality condition can be implemented in COMSOL MULTIPHYSICS scripts. Some examples illustrate the properties of our approach.

2. OPTIMALITY CONDITIONS FOR PROBLEMS WITH INEQUALITY CONSTRAINTS

Let an optimal control problem (OCP) be given as

$$(3) \quad \begin{aligned} \min j(y, u) &= \frac{\theta_\Omega}{2} \|y(T) - y_\Omega\|_{L^2(\Omega)}^2 + \frac{\theta_Q}{2} \|y - y_Q\|_{L^2(Q)}^2 + \frac{\theta_\Sigma}{2} \|y - y_\Sigma\|_{L^2(\Sigma)}^2 \\ &+ \frac{\kappa_Q}{2} \|u_Q\|_{L^2(Q)}^2 + \frac{\kappa_\Sigma}{2} \|u_\Sigma\|_{L^2(\Sigma)}^2 \end{aligned}$$

subject to the parabolic PDE

$$(4) \quad \begin{aligned} y_t - \nabla \cdot (\nabla A y) + a_0 y &= u_Q + f && \text{in } Q \\ \vec{n} \cdot \nabla y + \alpha y &= u_\Sigma + g && \text{on } \Sigma \\ y(0) &= y_0 && \text{in } \Omega \end{aligned}$$

and to the pointwise (box) constraints

$$(5) \quad y_a \leq \tau y + \lambda u_Q \leq y_b \text{ a.e. in } Q$$

or to the (lower) unilateral constraints²

$$(6) \quad y_c \leq \tau y + \lambda u_Q \text{ a.e. in } Q.$$

Here, let $\Omega \subset \mathbb{R}^N$, $N \in \mathbb{N}$, be a bounded domain with $C^{0,1}$ -boundary Γ if $N = 2$, and a bounded interval in \mathbb{R} if $N = 1$. Moreover, for $Q = \Omega \times (0, T)$, we consider the data $u_Q \in L^2(Q)$, $f \in L^\infty(Q)$, $u_\Sigma \in L^2(\Sigma)$, $g \in L^\infty(\Sigma)$, $\Sigma = \Gamma \times (0, T)$, and $y_0 \in C(\Omega)$. Further, $A = (a_{ij}(x))$, $i, j = 1, \dots, N$ is a symmetric matrix with $a_{ij} \in C^{1,\gamma}(\Omega)$, $\gamma \in (0, 1)$. It is assumed to satisfy the following condition of uniform ellipticity: There is an $m > 0$ such that

$$\lambda^\top A(x) \lambda \geq m |\lambda|^2 \quad \text{for all } \lambda \in \mathbb{R}^N \text{ and all } x \in \bar{\Omega}.$$

Moreover, functions $a_0 \in L^\infty(Q)$, $y_Q \in L^\infty(Q)$, $y_\Omega \in L^\infty(\Omega)$ are given. In the case of box-constraints, the functions $y_a, y_b \in C(\bar{Q})$ satisfy $y_a(x, t) < y_b(x, t)$ for all $(x, t) \in \bar{Q}$ and it holds $y_a(x, 0) < y_0 < y_b(x, 0)$ a.e. in Ω .

By the continuity of y_a and y_b , there is some $c_Q > 0$, such that

$$(7) \quad y_b(x, t) - y_a(x, t) \geq c_Q \quad \forall (x, t) \in \bar{Q}$$

holds. Moreover, we define the solution space

$$W(0, T) = \{y \in L^2(0, T; H^1(\Omega)) \mid y_t \in L^2(0, T, H^1(\Omega)^*)\}.$$

Theorem 2.1. *For any triple $(u_Q + f, u_\Sigma + g, y_0) \in L^2(Q) \times L^2(\Sigma) \times L^2(\Omega)$ the initial value problem (4) admits a unique solution $y \in W(0, T)$. It holds*

$$\|y\|_{W(0, T)} \leq c (\|u_Q + f\|_{L^2(Q)} + \|u_\Sigma + g\|_{L^2(\Sigma)} + \|y_0\|_{L^2(\Omega)}).$$

For the proof we refer to Wloka [21], or Lions [10].

Theorem 2.2. *Let Ω be a bounded domain with $C^{1,1}$ -boundary. Further let $u_Q + f \in L^p(Q)$, $u_\Sigma + g \in L^q(\Sigma)$ and $y_0 \in L^\infty(\Omega)$ be given. For every $p > N/2 + 1$ and $s > N + 1$, the weak solution of (2) belongs to $L^\infty(Q) \cap C([\delta, T] \times \bar{\Omega})$ for all $\delta > 0$. There is a constant c not depending on (u, f, g) , such that*

$$\|y\|_{L^\infty(Q)} \leq c (\|u_Q + f\|_{L^p(Q)} + \|u_\Sigma + g\|_{L^q(\Sigma)} + \|y_0\|_{L^\infty(\Omega)}).$$

If $y_0 \in C(\bar{\Omega})$, then $y \in C(\bar{Q})$.

²In this paper, we only consider unilateral constraints of lower type $y_c \leq \beta y + \gamma u$. The theory for upper constraints $\beta y + \gamma u \leq y_c$ is completely analogous.

Remark 2.3. In the case of boundary control, we have only $u_\Sigma + g \in L^2(\Sigma)$, so that the assumption $q > N + 1$ of Theorem 2.2 is not fulfilled. In the case of distributed control, for space dimension $N > 1$ the assumption $p > N/2 + 1$ is not fulfilled. In both cases, we do not have the necessary regularity of the state y . For that reason, to obtain optimality conditions or Lagrange multipliers at all, we have to *assume* that the optimal state belongs to $C(\bar{Q})$.

2.1. Control constraints. Setting $\tau = 0$ and $\lambda = 1$, the mixed control-state box-constraints (5) become pure control constraints $y_a \leq u \leq y_b$ a.e. in Q and the unilateral constraint (6) becomes $y_c \leq u$.

Theorem 2.4. Let u_Σ^* , u_Q^* be optimal solutions to problem (1) with associated optimal state y^* . The adjoint state p is the solution of the adjoint equation

$$\begin{aligned} -p_t - \nabla \cdot (\nabla A p) + a_0 p &= \theta_Q(y^* - y_Q) && \text{in } Q \\ \vec{n} \cdot \nabla p + \alpha p &= \theta_\Sigma(y^* - y_\Sigma) && \text{on } \Sigma \\ p(T) &= \theta_\Omega(y^*(T) - y_\Omega) && \text{in } \Omega. \end{aligned}$$

Further, u_Q^* and u_Σ^* hold the projection formulas

$$\begin{aligned} u_Q^*(x, t) &= P_{[y_a(x, t), y_b(x, t)]} \left\{ -\frac{1}{\kappa_Q} p(x, t) \right\} && \text{in } Q \\ u_\Sigma^*(x, t) &= P_{[y_a(x, t), y_b(x, t)]} \left\{ -\frac{1}{\kappa_\Sigma} p(x, t) \right\} && \text{on } \Sigma. \end{aligned}$$

The numerical treatment of control constrained problems is widely discussed in the literature, cf. [6],[3],[9], so we abstain from giving some examples.

2.2. Pure state constraints. Setting $\lambda = 0$ and $\tau = 1$, the constraints become pure state constraints $y_a \leq y \leq y_b$.

Theorem 2.5. Let $u^* \in L^2(Q) \times L^2(\Sigma)$ be the optimal solution of problem with associated optimal state $y^* \in C(\bar{Q})$. Then u^* and y^* fulfill together with the adjoint state p the adjoint equation

$$\begin{aligned} -p_t - \nabla \cdot (\nabla A p) + a_0 p &= \theta_Q(y^* - y_Q) - \mu_Q + \eta_Q && \text{in } Q \\ \vec{n} \cdot \nabla p + \alpha p &= \theta_\Sigma(y^* - y_\Sigma) - \mu_\Sigma + \eta_\Sigma && \text{on } \Sigma \\ p(T) &= \theta_\Omega(y^*(T) - y_\Omega) - \mu_\Omega + \eta_\Omega && \text{in } \Omega, \end{aligned}$$

the gradient equation

$$\kappa_Q p + u_Q^* = 0 \text{ a.e. in } Q, \quad \text{and} \quad \kappa_\Sigma p + u_\Sigma^* = 0 \text{ a.e. on } \Sigma,$$

and the complementary slackness conditions

$$\begin{aligned} \iint_Q (y^* - y_a) d\mu_Q(x, t) &= 0 && \iint_\Sigma (y^* - y_a) d\mu_\Sigma(x, t) = 0 \\ \iint_Q (y_b - y^*) d\eta_Q(x, t) &= 0 && \iint_\Sigma (y_b - y^*) d\eta_\Sigma(x, t) = 0 \\ \mu_Q(x, t) &\geq 0 \text{ a.e. in } Q && y(x, t) - y_a(x, t) \geq 0 \text{ a.e. in } \bar{Q} \\ \eta_Q(x, t) &\geq 0 \text{ a.e. in } Q && y_b(x, t) - y(x, t) \geq 0 \text{ a.e. in } \bar{Q} \\ \mu_\Sigma(x, t) &\geq 0 \text{ a.e. in } \Sigma && \\ \eta_\Sigma(x, t) &\geq 0 \text{ a.e. in } \Sigma && \end{aligned}$$

Note, that the Lagrange multipliers μ_Q , μ_Σ , η_Q , η_Σ , η_Ω , and η_Ω , if existent, are in general regular Borel measures. This lack of regularity motivates the regularization by mixed control-state constraints.

2.3. Mixed control-state constraints. Let $\lambda > 0$ and $\tau > 0$ be given. These mixed control-state constraints can be seen as model-given or in the case of $\tau \gg \lambda > 0$ as regularization of pure state constraints by perturbation of the state constraint by a small quantity of the control. This technique is well know under the term *Laurentiev regularization*. Here we scale the constraints such that $\tau = 1$, $\lambda > 0$.

Theorem 2.6. Let u^* be the optimal solution of problem with associated optimal state y^* . Then u^* and y^* fulfill together with the adjoint state p the adjoint equation

$$\begin{aligned} -p_t - \nabla \cdot (\nabla A p) + a_0 p &= \theta_Q(y^* - y_Q) - \mu_Q + \eta_Q && \text{in } Q \\ \vec{n} \cdot \nabla p + \alpha p &= \theta_\Sigma(y^* - y_\Sigma) - \mu_\Sigma + \eta_\Sigma && \text{on } \Sigma \\ p(T) &= \theta_\Omega(y^*(T) - y_\Omega) && \text{in } \Omega, \end{aligned}$$

the gradient equation

$$\begin{aligned}\kappa_Q p + u^* - \gamma(\mu_Q - \eta_Q) &= 0 \text{ a.e. in } Q \\ \kappa_\Sigma - \gamma(\mu_\Sigma - \eta_\Sigma) &= 0 \text{ a.e. on } \Sigma\end{aligned}$$

and the complementary slackness conditions

$$\begin{aligned}(y^* + \lambda u^* - y_a) \mu_Q &= 0 \text{ a.e. in } Q & (y^* + \lambda u^* - y_a) \mu_\Sigma &= 0 \text{ a.e. on } \Sigma \\ (y_b - \lambda u^* - y^*) \eta_Q &= 0 \text{ a.e. in } Q & (y_b - \lambda u^* - y^*) \eta_\Sigma &= 0 \text{ a.e. on } \Sigma \\ \mu_Q(x, t) &\geq 0 \text{ a.e. in } Q & y^*(x, t) + \lambda u^*(x, t) - y_a(x, t) &\geq 0 \text{ a.e. in } \bar{Q} \\ \eta_Q(x, t) &\geq 0 \text{ a.e. in } Q & y_b(x, t) - \lambda u^*(x, t) - y^*(x, t) &\geq 0 \text{ a.e. in } \bar{Q}. \\ \mu_\Sigma(x, t) &\geq 0 \text{ a.e. in } \Sigma \\ \eta_\Sigma(x, t) &\geq 0 \text{ a.e. in } \Sigma\end{aligned}$$

Here, the Lagrange multipliers μ_Q , μ_Σ , η_Q , and η_Σ are regular L^2 -functions.

2.3.1. *Problem case: state constraints given on the space-time domain and control given only on the boundary.* One standard problem is the following:

$$(8) \quad \min j(y, u) = \frac{\theta_Q}{2} \|y - y_Q\|_{L^2(Q)}^2 + \frac{\kappa_\Sigma}{2} \|u_\Sigma\|_{L^2(\Sigma)}^2$$

subject to the boundary controlled PDE

$$(9) \quad \begin{aligned}y_t - \nabla \cdot (\nabla A y) + a_0 y &= 0 & \text{in } Q \\ \vec{n} \cdot \nabla y + \alpha y &= \alpha u_\Sigma & \text{on } \Sigma \\ y(0) &= y_0 & \text{in } \Omega\end{aligned}$$

and to the pointwise constraints in the interior of the space-time domain

$$(10) \quad y_c \leq y \text{ a.e. in } Q$$

The Lagrange multiplier is usually a Borel measure on the space-time domain Q . The standard Lavrentiev regularization cannot be applied because the control u is not defined in Q . Here, the new approach in [19] (for an elliptic PDE) or [15] (for a parabolic PDE) will help to overcome this problem. The Lavrentiev-like regularization. We replace (8)–(10) by the problem

$$(11) \quad \min j(y, w, v) = \frac{\theta_Q}{2} \|y - y_Q\|_{L^2(Q)}^2 + \frac{\kappa_\Sigma}{2} \|\alpha w\|_{L^2(\Sigma)}^2 + \frac{\epsilon}{2} \|v\|_{L^2(Q)}^2$$

subject to the state equation

$$(12) \quad \begin{aligned}y_t - \nabla \cdot (\nabla A y) + a_0 y &= 0 & \text{in } Q \\ \vec{n} \cdot \nabla y + \alpha y &= \alpha^2 w & \text{on } \Sigma \\ y(0) &= y_0 & \text{in } \Omega,\end{aligned}$$

to the additional equation

$$(13) \quad \begin{aligned}-w_t - \nabla \cdot (\nabla A w) + a_0 w &= v & \text{in } Q \\ \vec{n} \cdot \nabla w + \alpha w &= 0 & \text{on } \Sigma \\ w(T) &= 0 & \text{in } \Omega\end{aligned}$$

and to the state constraints with modified Lavrentiev-type regularization³

$$(14) \quad y_c \leq y + \lambda v \text{ a.e. in } Q.$$

In [15] convergence for vanishing Lavrentiev parameters is shown if ϵ is chosen according to $\epsilon = c_0 \lambda^{1+c_1}$, $c_0 > 0$ and $0 \leq c_1 < 1$.

Theorem 2.7. *Let (y^*, v^*, w^*) be the optimal solution of (11)–(14). Then there exist adjoint states $p, q \in W(0, T)$, and a Lagrange multiplier $\mu_Q \in L^2(Q)$ such that the following first-order optimality conditions hold:*

³The idea behind this regularization is, to introduce an auxiliary distributed control v which is coupled with u by an adjoint equation, $u = S^* v$, where S denotes the solution operator of the state equation and S^* its adjoint. Here, w is the solution of the adjoint equation and u its trace. Cf. [15].

State and adjoint equation

$$(15) \quad \begin{aligned} y_t - \nabla \cdot (\nabla A y^*) + a_0 y^* &= 0 && \text{in } Q \\ \vec{n} \cdot \nabla y^* + \alpha y^* &= \alpha^2 w_\Sigma^* && \text{on } \Sigma \\ y^*(0) &= y_0 && \text{in } \Omega \end{aligned}$$

$$(16) \quad \begin{aligned} -p_t - \nabla \cdot (\nabla A p) + a_0 p &= \theta_Q (y^* - y_Q) - \mu_Q && \text{in } Q \\ \vec{n} \cdot \nabla p + \alpha p &= 0 && \text{on } \Sigma \\ p(T) &= 0 && \text{in } \Omega. \end{aligned}$$

Control and second adjoint equation

$$(17) \quad \begin{aligned} -w_t - \nabla \cdot (\nabla A w^*) + a_0 w^* &= -\frac{1}{\epsilon} q + \frac{\lambda}{\epsilon} \mu_Q && \text{in } Q \\ \vec{n} \cdot \nabla w^* + \alpha w^* &= 0 && \text{on } \Sigma \\ w^*(T) &= 0 && \text{in } \Omega \end{aligned}$$

$$(18) \quad \begin{aligned} q_t - \nabla \cdot (\nabla A q) + a_0 q &= 0 && \text{in } Q \\ \vec{n} \cdot \nabla q + \alpha q &= \alpha^2 (\kappa_\Sigma w_\Sigma^* + p) && \text{on } \Sigma \\ q(0) &= 0 && \text{in } \Omega. \end{aligned}$$

Gradient equation

$$(19) \quad \epsilon v^* + q - \lambda \mu_Q = 0 \text{ a.e. in } Q.$$

Complementary slackness conditions

$$(20) \quad \begin{aligned} (\mu_Q, y^* + \lambda v - y_c)_{L^2(Q)} &= 0 \\ \mu_Q &\geq 0 \text{ a.e. in } Q \\ y^* + \lambda v - y_c &\geq 0 \text{ a.e. in } Q \end{aligned}$$

The proof is given in [15]. Here, the Lagrange multiplier is a regular L^2 -function. Note, that the equations (17) and (18) are from the same type as the state equation (15) and the adjoint equation (16).

3. ALGORITHMS TO HANDLE STATE CONSTRAINTS

3.1. The barrier method. Barrier methods replace the inequality constraints by adding an arbitrary barrier (or penalty) term to the objective functional.

Definition 3.1. Let $z_i = z_i(y, u)$ be the implementation of the boundary conditions (5) or (6) i.e. $z_1 = \beta y + \gamma u - y_a$, $z_2 = y_b - \beta y + \gamma u$, or $z_3 = \beta y + \gamma u - y_c$. For all $q \geq 1$ and $\mu > 0$ the functions $g_i(z; \mu; q) : \mathbb{R}_+ \rightarrow \mathbb{R} \cup \{+\infty\}$ defined by

$$g_i(z; \mu; q) := \begin{cases} -\mu \ln(z_i) & : q = 1 \\ \frac{\mu^q}{(q-1)z_i^{q-1}} & : q > 1 \end{cases}$$

for $i = 1, 2, 3$ are called barrier functions of order q .

Definition 3.2. Let $G_{bi} := \{(y, u) \in Y \times U \mid y_a < \beta y + \gamma u < y_b\}$ and $G_{uni} := \{(y, u) \in Y \times U \mid y_c < \beta y + \gamma u\}$. We call G_{bi} and G_{uni} resp. the admissible set concerning the inequality constraints. Further, let

$$E := \{(y, u) \in Y \times U \mid (y, u) \text{ fulfill the state equation (4)}\}.$$

We define by

$$\chi_M(z) := \begin{cases} 0 & z \in M \\ \infty & \text{otherwise} \end{cases}$$

the indicator function on the set M .

We can now re-define our basic problems without any constraints. Let $g_i(z_i; \mu; q)$ be barrier functions to the given inequality constraints. Then we eliminate all constraints by defining the new problems

Algorithm 1 Path-following

```

Choose  $\mu_0$ ,  $0 < \sigma < 1$  arbitrary.
choose some starting values for  $y_k$ ,  $p_k$ 
while  $\mu_k > \text{eps}$ 
  solve the optimality condition
     $F(y_{k+1}, u_{k+1}, p_{k+1}; \mu_k) = 0$ 
  by Newtons method with starting value
     $(y_k, u_k, p_k)$  up to a accuracy  $\delta$ .
  If it fails, increase  $\sigma < 1$  and try again.
  set  $\mu_{k+1} = \mu_k \cdot \sigma$ ,  $k = k + 1$ ;
end
  
```

$$(21) \quad \min f_{bi}(y, u) = j(y, u) - \iint_Q \sum_{i \in I} g_i(z_i(y, u), \mu, q) dxdt + \chi_{bi}(y, u) + \chi_E(y, u)$$

(bilateral constraints) or

$$(22) \quad \min f_{uni}(y, u) = j(y, u) - \iint_Q \sum_{i \in I} g_i(z_i(y, u), \mu, q) dxdt + \chi_{uni}(y, u) + \chi_E(y, u)$$

(unilateral constraint). Obviously, these are unrestricted problems. First we observe that every pair (y, u) that holds $f(y, u) < \infty$ is feasible with respect to the inequality constraints and the equality constraints. The functional f_{bi} and f_{uni} are coercive, convex, and lower semi-continuous. This optimal control problem is equivalent to the problem (1) with pure state constraints. The following theorem from Schiela [17] yields the existence of a unique minimizer for problems (21) and (22).

Theorem 3.3. *Let $f : Z = (Y, U) \rightarrow \bar{\mathbb{R}}$ be a proper, convex, lower semi-continuous functional of the form (21) or (22), resp. Let f be coercive for all $\mu \leq \mu_0$. Further, let E be a sequentially compact subspace of Z .*

The problems (21) and (22) have for every $\mu > 0$ a unique minimizer $z_\mu = (y_\mu, u_\mu)$. Moreover, z_μ is strictly feasible almost everywhere in Q and bounded in Z uniformly in $\mu \in [0, \mu_0]$.

The next theorem provides necessary first order optimality conditions. We write $Ly = u$, where L is the differential operator associated with the PDE (4).

Theorem 3.4. *Let the general assumptions given in Theorem 3.3 hold and let $z = (y, u)$ be the unique minimizer of (21) or (3.3).*

Then there are $(j_y, j_u) = j \in \partial j(z)$, $m \in \partial g(z(y, u), \mu, q) \in Y^$, and $p \in \text{dom} L^*$ such that*

$$\begin{aligned} j_y + m + L^*p &= 0 \\ j_u + g'(z(y, u); \mu; q) &= 0 \\ Ly - u &= 0 \end{aligned}$$

holds. If y is strictly feasible, then $\partial g = g'(z(y, u)z'(y, u))$ and m is unique. If $\partial j(z)$ contains only one element, and $\mu > 0$, then m and p are unique in Y^ and U^* , respectively.*

For a detailed presentation we refer again to [17], cf. Proposition 4.2 and Theorem 4.3. The differential operator L^* is nothing else but the usual adjoint equation.

We use the last theorems to implement the path-following Algorithm 1.

Note 3.5. Theorem 3.3 provides for fixed μ_k a unique solution. To find that solution, we have to solve the optimality conditions given by Theorem 3.4. In the spirit of [14], we want to do this by using COMSOL MULTIPHYSICS solving the optimality conditions, i.e. a system of non-linear coupled PDEs, by Newtons method. Unfortunately, we have no information concerning the convergence radius of Newtons method, so we cannot ensure the convergence of the path-following method. However, if we found a solution for some μ_0 , we can decrease the path parameter μ by setting $\mu_k = \sigma \mu_{k-1}$. In the worst case, this σ will almost be one so that the algorithm runs into emptiness.

For further details we refer to [20, 16].

3.2. The projection method. Our projection method replaces the complementary slackness conditions by a projection. In some sense, this is an implementation of the well known active set strategy. One can show that the complementary slackness conditions (20) are equivalent to

$$\mu_Q = \max \{0, \mu_Q + c(y_c - \lambda v^* - y^*)\},$$

cf. [7] for an arbitrarily chosen fixed $c > 0$. Equation (19) yields $\mu_Q = \frac{1}{\lambda}(\epsilon v^* + q)$. Choosing $c = \frac{\epsilon}{\lambda^2} > 0$ as in [19], we obtain a projection formula for the Lagrange multiplier

$$(23) \quad \mu_Q = \max \left\{ 0, \frac{1}{\lambda}q - \frac{\epsilon}{\lambda^2}(y^* - y_c(x, t)) \right\} \text{ a.e. in } Q.$$

Now, we have to solve an optimality system consisting of the PDEs (15), (16), (17), and (18), and the projection (23). In Section 4.1.2 we present some details of the implementation of these method in our COMSOL MULTIPHYSICS-code.

3.3. The penalty method by Ito and Kunisch. The penalty method replaces the state constraint by a modified objective functional. We consider only the case with state constraints given on the space-time domain Q . The problem reads now

$$\begin{aligned} \min j(y, u) = & \frac{\theta_\Omega}{2} \|y(T) - y_\Omega\|_{L^2(Q)}^2 + \frac{\theta_Q}{2} \|y - y_Q\|_{L^2(Q)}^2 + \frac{\theta_\Sigma}{2} \|y - y_\Sigma\|_{L^2(\Sigma)}^2 \\ & + \frac{\kappa_Q}{2} \|u\|_{L^2(Q)}^2 + \frac{\kappa_\Sigma}{2} \|u\|_{L^2(\Sigma)}^2 + \frac{1}{2\gamma} \left(\iint_Q |\gamma(y_a - y) + \bar{\mu}_Q|^2 dxdt + \iint_Q |\gamma(y - y_b) + \bar{\eta}_Q|^2 dxdt \right) \end{aligned}$$

subject to the state equation (4).

Here, $\bar{\eta}_Q, \bar{\mu}_Q$ are arbitrary functions that belong to $L^2(\Omega)$ and $\gamma \in \mathbb{R}, \gamma \gg 1$ is a regularization parameter. We obtain the Moreau-Yosida regularized multipliers

$$\begin{aligned} \mu_Q &= \max\{0, \bar{\mu}_Q + \gamma(y_a - y)\} \\ \eta_Q &= \max\{0, \bar{\eta}_Q + \gamma(y - y_b)\}. \end{aligned}$$

Without proof we consider the optimality system

$$(24) \quad \begin{aligned} y_t - \nabla \cdot (A \nabla y) &= u_Q + f & \text{in } Q & & -p_t - \nabla \cdot (A \nabla p) &= \theta_Q(y - y_Q) + \eta_Q - \mu_Q & \text{in } Q \\ \vec{n} \cdot \nabla y + \alpha y &= \alpha(u_\Sigma + g) & \text{on } \Sigma & & \vec{n} \cdot \nabla p + \alpha p &= \theta_\Sigma(y - y_\Sigma) & \text{on } \Sigma \\ y(0) &= y_0 & \text{in } \Omega & & y(T) &= \theta_\Omega(y(T) - y_\Omega) & \text{in } \Omega \\ \kappa_Q u + p &= 0 & \text{in } Q & & \mu_Q &= \max\{0, \gamma(y_a - y)\} \\ \kappa_\Sigma u + p &= 0 & \text{on } \Sigma & & \eta_Q &= \max\{0, \gamma(y - y_b)\}, \end{aligned}$$

where we choose $\bar{\eta}_Q \equiv \bar{\mu}_Q \equiv 0$. For details see [8].

4. NUMERICAL TESTS USING COMSOL MULTIPHYSICS

4.1. A boundary controlled problem. Our first example was originally given by Betts and Campbell in [4].

Let $\Omega = [0, 1]$ and the time interval $I = (0, 5)$ be given. The problem formulation reads as follows

$$\min j(y, u) = \frac{1}{2} \|y - y_d\|_Q^2 + \frac{\kappa}{2} \|u\|_{L^2(\Sigma)}^2$$

subject to

$$(25) \quad \begin{aligned} y_t - \Delta y &= 0 & \text{in } Q \\ y &= u & \text{on } \Sigma \\ y(0) &= 0 & \text{in } \Omega \end{aligned}$$

and the pointwise state constraints

$$y_c \leq y \quad \text{a.e. in } Q.$$

The state constraint is given by $y_c(x, t) = \sin(x)(\sin(\pi t/5)) - 0.7$, the function $y_d \equiv 0$ and let κ be given as 10^{-3} .

The Dirichlet-boundary condition is difficult in two ways: Neither can they be handled by finite element methods in the usual way, cf. [2], nor are optimality conditions derived easily.

A possible way to overcome this problem is to approximate the Dirichlet-boundary conditions by Robin boundary conditions: For some $\alpha \gg 1$ arbitrary chosen, we replace (25) by $\vec{n} \cdot \nabla y + \alpha y = \alpha u$ on Σ . Some results concerning convergence analysis can be found in [1].⁴ We use Robin boundary conditions for a correct finite elements implementation of the state equation as well as for a correct implementation of the adjoint equation. We choose $\alpha = 10^3$. In the following, we assume that there is a continuous optimal state which ensures the existence of optimality conditions wherever we consider an unregularized problem.

⁴COMSOL MULTIPHYSICS uses this technique for solving Dirichlet boundary problems by default. In this way it is possible to implement the "wrong given" boundary conditions directly in COMSOL MULTIPHYSICS, where it will be corrected by using a Robin formulation with a well-chosen parameter α internally.

4.1.1. *The barrier method.* Theorem 3.4 provides a more or less abstract formulation of the optimality system. To receive an implementable optimality condition, e.g. a system of PDEs, we use a formal Lagrange technique. We define the Lagrange function

$$L(y, u, p; \mu) = j(y, u) - \iint_Q (y_t - \Delta y)p \, dxdt - \iint_\Sigma \vec{n} \cdot \nabla y + \alpha(y - u)p \, dxdt - \iint_Q \frac{\mu^2}{y - y_c} \, dxdt.$$

Formal derivation yields the optimality system

$$\begin{aligned} -p_t - \Delta p &= y - y_d - \frac{\mu^2}{(y - y_c)^2} && \text{in } Q && y_t - \Delta y &= 0 && \text{in } Q \\ \vec{n} \cdot \nabla p + \alpha p &= 0 && \text{on } \Sigma && \vec{n} \cdot \nabla y + \alpha y &= -\frac{\alpha}{\kappa_Q} p && \text{on } \Sigma \\ p(T) &= 0 && \text{in } \Omega && y(0) &= y_0 && \text{in } \Omega \end{aligned}$$

where we replaced the control by the adjoint p using the relation $\kappa u + p = 0$ a.e. on Σ . With a formal re-implementation of an approximation of the Lagrange multiplier η_μ by $\eta_\mu := \frac{\mu^2}{(y - y_a)^2}$, we have the additional relations $\eta_\mu(y - y_a)^2 = \mu^2$ and $\eta_\mu > 0$ a.e. in Q , and $(y - y_a)^2 > 0$ a.e. in Q . In the following excerpts of the COMSOL MULTIPHYSICS-code we show how this condition is implemented by using a complementary function of Fischer-Burmeister type. We chose $eps = 0.0008$ and $\sigma = 1/2$. In this paper, we present only the essentials of the COMSOL MULTIPHYSICS-script we used to solve the examples. For a more detailed presentation we refer to [14] and the web-side

www.math.tu-berlin.de/Strategies-for-time-dependent-PDE-control.html

Definition of the complementary function:

```
fem.equ.ga = { { {'-yx' '0'} {'-px' '0'} {'0' '0'} } };
fem.equ.f = { {'-ytime'...
              'ptime+y-eta'...
              '(y-y_a(x,time))^2+eta...
              '-sqrt(eta^2+(y-y_a(x,time))^4+2*mu^2)'} } };
```

The boundary conditions:

```
fem.bnd.r = {{ 'y' '0' 'eta' };
             { '0' '0' 'eta' };
             { '0' 'p' 'eta' } };
fem.bnd.g = {{ '0' '0' '0' };
             { '-alpha/kappa*p-alpha*y' '-alpha*p' '0' };
             { '0' '0' '0' } };
```

The heart of the program, the path following loop:

```
fem = adaption(fem, 'ngen', 1, 'Maxiter', 50, 'Hnlin', 'on');
mu0=1e-1;
while mu0>0.0008,
    mu0=mu0*0.5;
    fem.const{4} = num2str(mu0);
    fem.xmesh = meshextend(fem);
    fem = femnlin(fem, 'init', fem.sol, ...
                 'out', 'fem', 'Hnlin', 'off', 'Maxiter', 50);
end
```

4.1.2. *The projection method.* Most of the code is the same as for the barrier method, we briefly sketch the differences and give some hints for implementing the regularized optimality system.

The definition of the variables: all PDE variables are on second order, the Lagrange multiplier is discretized with linear finite elements.

```
fem.dim = {'y' 'w' 'p' 'q' 'mu'};
fem.shape = [2 2 2 2 1];
% parameters:
fem.const = {'alpha' '1e+3' 'kappa' '1e-3'...
             'lambda' '1e-6' 'epsilon' '1e-9'};
```

The definition of the optimality system. In the last line of the definition of f we implement the projection formula.

```

% coefficients + rhd side:
fem.globalexpr = {'v' '-1/epsilon*q+lambda/epsilon*mu'};
fem.equ.ga = {{{'-yx' '0'}
               {'-wx' '0'}
               {'-px' '0'}
               {'-qx' '0'}
               {'0' '0'}}};
fem.equ.f = { {'-ytime' 'wtime+v' 'ptime+y-mu' '-qtime'...
              'mu-max(0,1/lambda*q+epsilon/lambda^2...
              *(ya(x,time)-y))' } };

```

Next, the definition of the boundary conditions:

```

fem.bnd.r = {{{'y' '0' '0' 'q' '0'};
              {'0' '0' '0' '0' '0'};
              {'0' 'w' 'p' '0' '0'} };
fem.bnd.g = {{{'0' '0' '0' '0' '0'};
              {'alpha^2*w-alpha*y' '-alpha*w' '-alpha*p'...
              '-alpha*q+nu*alpha^2*w+alpha^2*p' 0};
              {'0' '0' '0' '0' '0'}}};

```

The problem was solved by one call of the function `adaption`. Note that we carry out our numerical experiments with the choice of $\lambda = 10^{-6}$ and $\epsilon = 10^{-9}$.

4.1.3. *The penalty method.* Analogously to the other examples, we use the gradient equation to replace the control u_Σ by $-\frac{\alpha}{\kappa_\Sigma}p$.

Altogether, we have to change the code only in four lines. First, we have to define the penalty parameter

```

% parameters:
fem.const = {'alpha' '1e+3' 'kappa' '1e-3' 'gamma' '1e+3'};

```

The definition of the right-hand-side reads now

```

fem.equ.f = { {'-ytime' 'ptime+y-mu' '-mu+max(0,gamma*(ya(x,time)-y))' } };

```

Finally, we have to write the boundary conditions as

```

fem.bnd.r = { {'y' '0' 'mu'};
              {'0' '0' 'mu-max(0,gamma*(ya(x,time)-y))' };
em.bnd.g = { {'0' '0' '0'};
              {'-alpha*y-alpha^2/kappa*p' '-alpha*p' '0'};
              {'0' '0' '0'} };

```

In our experiments we chose $\gamma = 10^3$. For further details see

<http://www.math.tu-berlin.de/Strategies-for-time-dependent-PDE-control/>

4.1.4. *Results.* There is no analytically given solution for the Betts-Campbell problem, so we can only compare solutions computed by different numerical methods. In the barrier method, we compute a solution for μ_0 on an adaptive mesh before we enter the path following loop. Obviously, the adaption process leads to very small mesh sizes near the boundaries at time t_0 and where the distance between the state y and the bound y_c is small, i.e. the bound y_c is almost active. In the projection method, the grid-adaption process is done in the same call of the function `adaption` that solves the complete problem. In adaption we set the number of new grid generations `ngen` to two. Moreover, when applying the projection method and the penalty method, we use the option `hnl` (“highly nonlinear problem”), which results in a smaller damping factor in Newton’s method. Figure 1 shows both adaptively refined meshes.

Figure 2 shows the control $u(\pi, t)$ computed by different numerical methods. For a comparison of the results, we computed two reference solutions by two different methods. First we use the space-time-adaptive interior point solver described in [16], adapted to boundary problems, and second, we use the quadratic programming solver from the MOSEK⁵ package. MOSEK offers an interface to MATLAB⁶ that emulates MATLAB’s `quadprog` function (from the optimization toolbox). For that, we have to formulate our problem as a discrete optimization problem of the form

$$\min z^\top \left(\frac{1}{2} H \right) z + b^\top z$$

⁵MOSEK uses an interior point solver. It is an implementation of the homogeneous and self-dual algorithm. For details see the MOSEK manual [13] and the referred literature there. In fact, both reference solvers are interior point solvers, but the solver `ip-adaptive` solves the optimality condition given as PDE (“first optimize, then discretize approach”), MOSEK solves the discrete optimization problem (“first discretize, then optimize approach”). See the discussion of the different approaches e.g. in [5].

MOSEK is a registered trademark of MOSEK ApS

⁶MATLAB is a registered trademark of THE MATHWORKS, Inc.

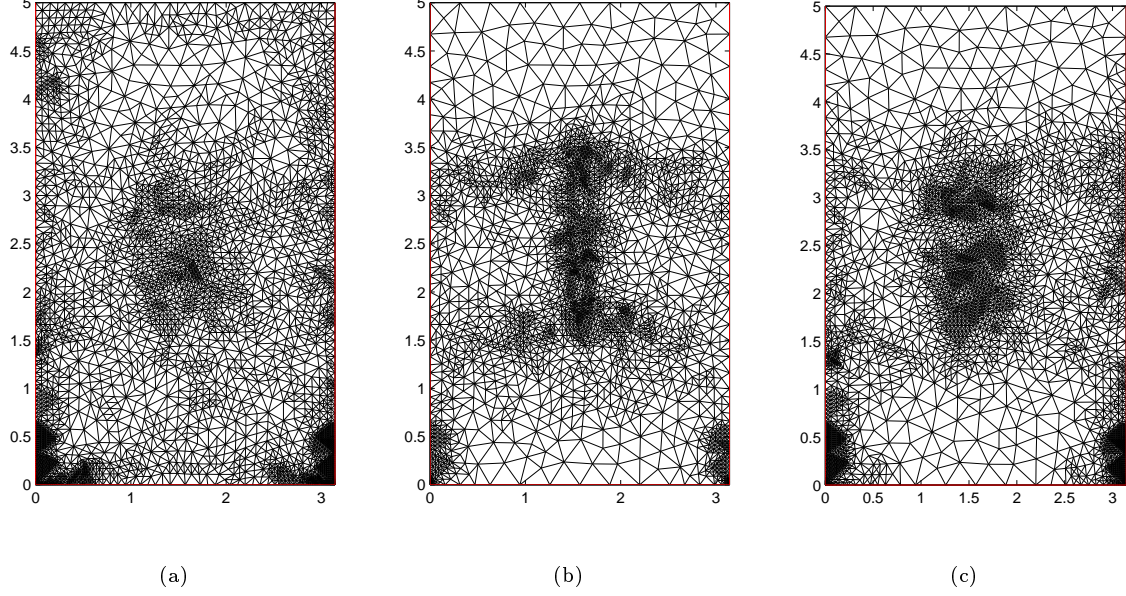


FIGURE 1. Adaptive meshes: barrier method (a), projection method (b), and penalty method (c). All meshes computed by COMSOL MULTIPHYSICS' adaption method with one new grid generation. The necessity for mesh refinement on the boundary at time $t \approx 2$ was detected by COMSOL MULTIPHYSICS' mesh-refinement algorithm only in the penalty method.

subject to

$$\begin{aligned} A_{eq}z &= b_{eq} \\ A_{in}z &\leq b_{in}. \end{aligned}$$

Let $(0 = t_0, \dots, t_k, \dots, t_n = T)$ be a discrete time interval and $y_k = y(t_k)$, $u_k = u(t_k)$. Let the space Ω be discretized and let M be the usual mass matrix associated with linear finite elements.

We set $z = (y_0 - y_d(t_0), \dots, y_n - y_d(T), u_0, \dots, u_n)^\top$, $b = 0$, and

$$H = \begin{pmatrix} 0 & \dots & 0 \\ & 0 & \\ & & \ddots & \vdots \\ & & & M \\ \vdots & & & & Q & 0 \\ & & & & 0 & \ddots & 0 \\ 0 & \dots & & & 0 & & Q \end{pmatrix}.$$

The matrix A_{eq} implements the state equation as described in [16]. We assume that we have given the stiffness matrix K , the mass matrix M_{a_0} associated with the coefficient a_0 , the matrix that contains the boundary integral Q and the right-hand-side vector G . Further, let the derivative with respect to the time y_t be approximated by backward finite differences, e.g. by the implicit Euler formula. $y_t(t_{k+1}) = \frac{1}{\delta t_{k+1}}(y(t_{k+1}) - y(t_k))$.

We get the recursive formula

$$\begin{aligned} (\delta t_{k+1} + 1)M + \delta t_{k+1}(K + Q)y_{k+1} - My_k - \delta t_{k+1}Qu_{k+1} &= 0 & \text{for } k = 1, \dots, n \\ y_0 &= y(0). \end{aligned}$$

Now, solving the state equation can be seen as matrix multiplication

$$A_{eq}z = b_{eq}$$

with

$$A_{eq} = \begin{pmatrix} E & 0 & \dots & 0 & 0 & 0 & \dots & 0 \\ -M & (\delta t_1 + 1)M + \delta t_1(K + Q) & 0 & \vdots & 0 & \delta t_1 Q & 0 & \vdots \\ 0 & \ddots & \ddots & 0 & \vdots & 0 & \ddots & 0 \\ 0 & 0 & -M & (\delta t_n + 1)M + \delta t_n(K + Q) & 0 & \dots & 0 & \delta t_n Q \end{pmatrix}$$

and

$$b_{eq} = \begin{pmatrix} y_0 \\ -(\delta t_1 + 1)M + \delta t_1(K + Q)y_d(t_1) \\ \vdots \\ -(\delta t_n + 1)M + \delta t_n(K + Q)y_d(t_n) \end{pmatrix}.$$

The mixed control-state constraints are implemented by $A_{in}z \leq b_{in}$ within the matrix

$$A_{in} = - \begin{pmatrix} E & 0 & 0 & \lambda E & 0 & 0 \\ 0 & \ddots & 0 & 0 & \ddots & \vdots \\ 0 & 0 & E & 0 & \dots & \lambda E \end{pmatrix}$$

and the vector $b_{in} = -((y_c)_0 + y_d(t_0), \dots, y_c(T) + y_d(T))^T$. In contrast to `quadprog` from MATLAB's optimization toolbox, MOSEK can handle sparse matrices so that the limitation of the number of unknowns is lifted.

Note, that the solutions computed by `quadprog` and `ip-solve` belong to the unregularized problem formulation since measures do not appear in the optimality systems of the discrete problems. Figure 2 shows the results for the Betts-Campbell heat transfer problem computed by different solution methods. Note that a typical behavior of barrier and interior point methods can be observed: Since the lower bound is a concave function, the methods tend to react more strongly in the first part in order to satisfy $y > \tau(\mu) + y_c$ for a $\tau(\mu) > 0$, where μ is the path parameter of the barrier/interior point methods. On the other hand, they react more smoothly in the second part where the values of the bound are decreasing. In some sense, barrier and interior point methods react to obstacles earlier than the active-set-based methods.

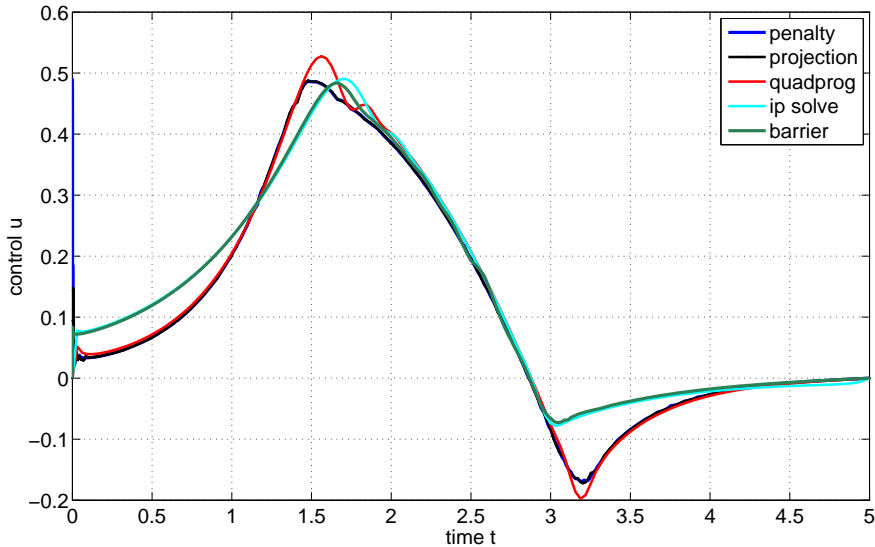


FIGURE 2. Solutions of the Betts-Campbell problem. Controls u_h computed by the penalty method (blue), by the projection method (black), by the MOSEK solver `quadprog` (red), by an adaptive interior-point solver (light blue), and by the barrier method (green).

A question of special interest is the behavior of the Lagrange multipliers. In the case of the Betts-Campbell example, the Lagrange multiplier seems to be a regular Borel measure.

	Barrier meth.	Projection method	Penalty method			quadprog	ip-solve
hauto				h	δt	$J(y, u)$	$J(y, u)$
7	0.2354	0.2260	—*	0.3142	0.2500	0.2611	0.2661
6	0.2374	0.2261	0.2212	0.1571	0.1250	0.2462	0.2512
5	0.2382	0.2261	0.2212	0.0785	0.0625	0.2393	0.2441
4	0.2382	0.2261	0.2212	0.0393	0.0393	0.2362	0.2412
3	0.2382	0.2261	0.2212	0.0196	0.0156	0.2346	0.2396

TABLE 1. Values of J computed by the barrier method and the projection method. For comparison, we give results computed by an interior point solver and by quadprog. *No convergence for raw initial grids.

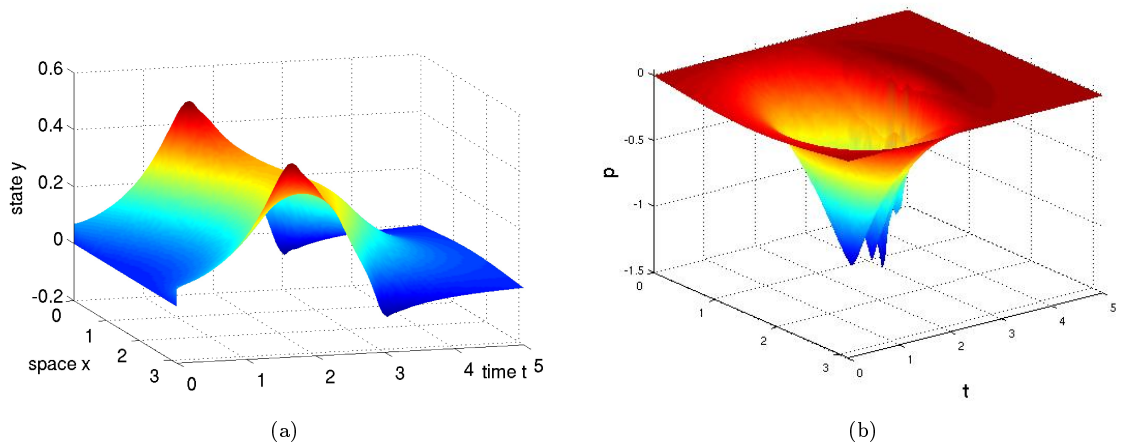


FIGURE 3. Example 1, Optimal state (a) and adjoint state (b), computed by the barrier method.

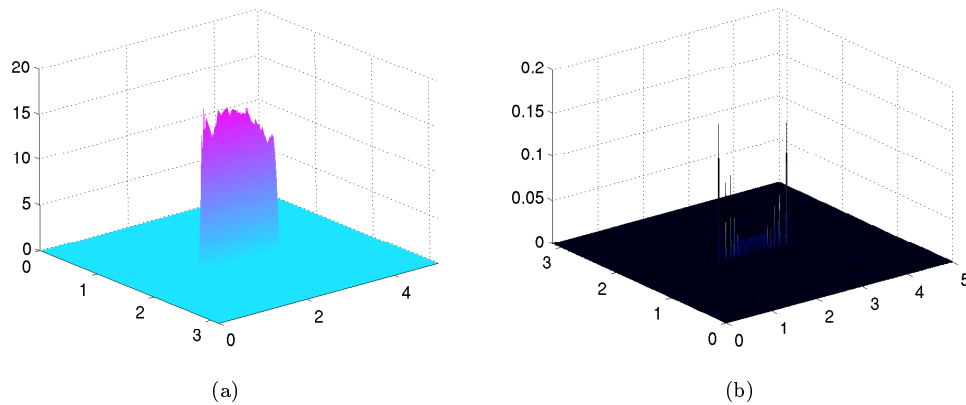


FIGURE 4. Lagrange Multiplier to the state constraint computed by the projection method (a) and by quadprog (b). The effects of the Lavrentiev-like regularization is obvious: the multiplier to the right looks like a measure, the left one is rather smooth. In the right figure, the edges of the grid are projected onto the graph. It is necessary to see more than two blue peaks.

4.2. Distributed control with state constraints. Our second example is taken from [16], Example 7.2. Again, there is no given analytical solution so we can only compare numerically computed solutions. The problem is given by

$$\min J(y, u) := \frac{1}{2} \|y(T) - y_d\|_{L^2(\Omega)}^2 + \frac{\kappa}{2} \|u\|_{L^2(Q)}^2$$

subject to

$$\begin{aligned} y_t - \Delta y &= u && \text{in } Q, \\ \partial_n y + 10y &= 0 && \text{on } \Sigma, \\ y(0) &= y_0 && \text{in } \Omega, \end{aligned}$$

and to the state constraint

$$y \geq y_a := \min\{-100(t(t-1) + x(x-1)) - 49.0, 0.5\} \quad \text{a.e. in } Q.$$

We choose $\Omega = (0, 1) \subset \mathbb{R}^1$, $T = 1$. Further, let $y_d \equiv 0$ and $y_0 = \sin(\pi x)$ be given. Obviously, this problem fits in our general setting with $\alpha = 10$.

4.2.1. *The barrier method.* The program is very similar to the one in the first example. We define the constraint in the usual way:

```
fcons{1}.type='inline';
fcons{1}.name='y_a(x,time)';
fcons{1}.expr='min(-100*(time*(time-1)+x*(x-1))-49,0.5)';
```

In contrast to the first example, the observation $\|y(T) - y_d\|_{L^2(\Omega)}$ works only on $\Omega \times \{T\}$, which results in a different end-condition in the adjoint equation: with $y_d \equiv 0$, we set $p(T) = y$. We define the optimality system:

```
fem.equ.ga = { { '-yx' '0' }
               { '-px' '0' }
               { '0' '0' } } };
fem.equ.f = { '-ytime-1/kappa*p' ...
              'ptime-eta'...
              '(y-lambda/kappa*p-y_a(x,time))...
              +eta-sqrt(eta^2+...
              (y- lambda/kappa*p-y_a(x,time))^2+2*mu)'} };
% boundaries: 1:t=0,2:x=pi,3:t=5,4:x=0
fem.bnd.ind = [1 2 3 2];
% boundary conditions:
fem.bnd.r = { {'y-y0(x)' '0' 'eta'};
              {'0' '0' 'eta'};
              {'0' 'p-y' 'eta'} };
fem.bnd.g = { {'0' '0' '0'};
              {'-alpha*y' '-alpha*p' '0'};
              {'0' '0' '0'} };

```

The last three rows in the definition of `fem.equ.f` define the Fischer-Burmeister complementary function. The rest of the code is the same as in Example 1. We choose $\epsilon = 10^{-5}$ and $\sigma = 1/2$.

4.2.2. *The projection method.* The parameters of the method are defined in the line

```
fem.const = {'alpha' '1e+1' 'lambda' '1e-3' 'kappa' '1e-3'};
```

The only difference to the implementation of the barrier method is the definition of `fem.equ.f`:

```
fem.equ.f = { '-ytime-1/kappa*p' ...
              'ptime-eta'...
              'eta-max(0,1/kappa*p+lambda/kappa^2*(y_a(x,time)-y))'} };

```

4.2.3. *The penalty method.* In the penalty method, we set $\alpha = 10$, $\kappa = 10^{-3}$, and $\gamma = 10^3$.

For implementing the penalty method we replace in the code of the projection method the projection by the penalty-function:

```
fem.equ.f = { {'-ytime-alpha^2/kappa*p'...
              'ptime-mu'...
              '-mu+max(0,gamma*(ya(x,time)-y))'} };

```

For a presentation of the complete source-code of all COMSOL MULTIPHYSICS-scripts we refer again to our web page

<http://www.math.tu-berlin.de/Strategies-for-time-dependent-PDE-control/>

4.2.4. *Results.* In Figure 5, we present the optimal state and the optimal control computed by the barrier method, cf. Figure 2 in [16].

As in the first example, we compared the solution of both methods with a solution computed by an interior point solver and a solution computed by the function `quadprog` provided by the package MOSEK. In this example, we refined the initial grid only once. The option `hnlm on` is used for all methods.

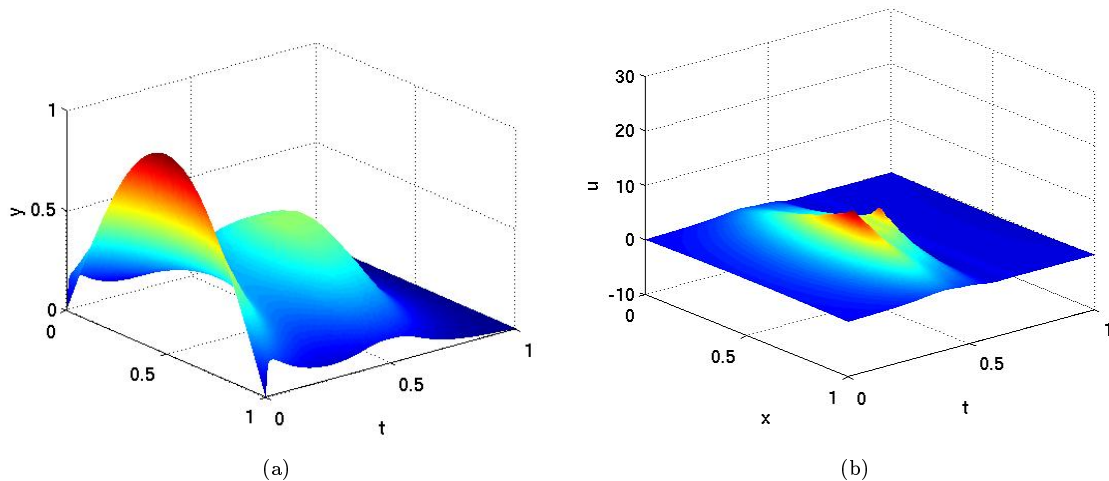


FIGURE 5. Optimal state (a) and optimal control (b)

	Barrier method	Projection method	Penalty method		ip-solve	quadprog
hauto	$J(y, u)$	$J(y, u)$	$J(y, u)$	h^*	$J(y, u)$	$J(y, u)$
5	0.0012354	0.0012475	0.0012754	0.1000	0.0012137	0.0012206
4	0.0012401	0.0012505	0.0012780	0.0667	0.0011921	0.0011607
3	0.0012427	0.0012430	0.0012703	0.0400	0.0012249	0.0012649
2	0.0012570	0.0012418	0.0012696	0.0250	0.0012327	0.0012729
1	0.0012590	0.0012419	0.0012696	0.0167	0.0012357	0.0012899

TABLE 2. Values of J by the barrier method and the projection method. For comparison, we give results computed by an interior point solver with time-adaptivity and by quadprog. *quadprog: time step-size chosen as half of space mesh-size. ip-solve: adaptive time step-size between $6.1451 \cdot 10^{-4}$ and 0.0839.

5. CONCLUSION AND OUTLOOK

As shown in [14] for the unconstrained case, the finite element package COMSOL MULTIPHYSICS can be used also for solving optimal control problems with state constraints. Again, a knowledge about the optimality system for the given problem is necessary. From the theoretical point of view, the handling of the state constraints and their associated Lagrange multipliers is the most difficult problem. To avoid measures in the optimality systems, we apply different regularization techniques in order to justify the use of standard FEM discretizations.

To handle (state)-constraints algorithmically, three approaches are considered. First, we implement a barrier method by adding a logarithmic or rational barrier term to the objective functional. The resulting algorithm is a classical (iterative) path following interior point method. Here, in every step a call of femnlin is necessary. On the other hand, the self-regularity of barrier methods permits to pass the Lavrentiev regularization if the order of the rational barrier function is high enough.

Second, via Lavrentiev and Lavrentiev-like regularization we arrive at a projection formula for the Lagrange multiplier which leads to an interpretation of the active set strategy as a (semi-smooth) Newton method. The resulting algorithm solved the problem by one call of adaption or femnlin respectively.

Third, we applied a Moreau-Yosida regularization method which can be interpreted as a penalization method which can be easily implemented with the help of the maximum function. We point out that we used fixed regularization parameters since we are not interested in the convergence behavior of these methods. It is beyond the scope of this paper to analyze the choice of regularization parameters in more detail. We refer for example to [12], where the influence of the Lavrentiev regularization parameter was examined. Instead our main point was to show the implementability in COMSOL MULTIPHYSICS of the regularization techniques.

We confirm our results by computing reference-solutions by two well-proven programs – an interior point solver based on a formulation of the optimality system as PDE and a quadratic programming solver MOSEK. All methods produce similar results in a variety up to ten percent. The difference in the results are a combination of

discretization and regularization effects. Therefore we cannot directly compare the controls defined on different grids, but we may expect that a well chosen combination of discretization parameters and parameters inherent to the solution technique such as Lavrentiev parameter, the penalty parameter, or the path parameter in the interior point method, results in a closer approximation of the “real” solution.

All together, COMSOL MULTIPHYSICS has the capability of solving optimal control problems with inequality constraints and offers an efficient alternative for solving such problems by an integrated modeling and simulation environment.

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