Solving Time-Dependent Optimal Control Problems in Comsol Multiphysics

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Abstract: We use COMSOL Multiphysics to solve time-dependent optimal control problems for partial differential equations whose optimality conditions can be formulated as a PDE. For a class of linear-quadratic model problems we summarize known analytic results on existence of solutions and first order optimality conditions that exhibit the typical feature of time-dependent control problems, namely the fact that a part of the optimality system has to be integrated backward in time. We present a strategy that is based on the treatment of the coupled optimality system in the space-time cylinder. Numerical examples show advantages and limits of the usage of COMSOL Multiphysics and of our approach.

Keywords: Optimal control of PDEs, finite element method, COMSOL Multiphysics.

1 Introduction

Optimal control problems subject to time-dependent partial differential equations are challenging from the viewpoint of mathematical theory and even more so from numerical realization. Essentially, there are two different approaches to solve such problems. The first one is the so-called "Discretize then Optimize" strategy, where the optimal control problem is transformed into a nonlinear programming problem by discretization. The second one is the function space based "Optimize then Discretize" strategy, that is based on developing optimality conditions in function spaces that are discretized and solved.

For certain classes of problems it is possible to derive optimality conditions in PDE form, and the latter strategy then involves solving systems of PDEs. It hence suggests itself to apply specialized PDE software to solve these systems. In this paper, we aim at applying COMSOL Multiphysics for optimization, taking advantage of the built-in routines to define, discretize and solve stationary and time-dependent PDEs via the finite element method.

We consider simple model problems either with distributed control consisting of the objective functional

$$J_Q(y,u) = \frac{1}{2}\int_Q (y-y_d)^2 + \kappa u^2 \, dxdt, \quad (1)$$

and the parabolic PDE with distributed control

$$\left.\begin{array}{rcll} y_t - \Delta y &=& u & \text{in } Q \\ \partial_n y + \alpha y &=& g & \text{on } \Sigma \\ y(t=0) &=& y_0 & \text{in } \Omega \end{array}\right\}, \quad (2)$$

or boundary control problems with objective functional

$$J_\Sigma(y,u) = \frac{\kappa}{2}\int_Q (y-y_d)^2 \, dxdt + \frac{\kappa}{2}\int_\Sigma u^2 \, dsdt \quad (3)$$

and the parabolic PDE with boundary control

$$\left.\begin{array}{rcll} y_t - \Delta y &=& f & \text{in } Q \\ \partial_n y + \alpha y &=& u & \text{on } \Sigma \\ y(t=0) &=& y_0 & \text{in } \Omega \end{array}\right\}. \quad (4)$$

Assumption 1. In this setting, $\Omega \subset \mathbb{R}^N$, $N = 1, 2$, is a spatial domain with sufficiently smooth boundary $\partial\Omega$, $(0,T)$ is a non-empty time interval, $\Sigma := \partial\Omega \times (0,T)$, and

$Q := \Omega \times (0,T)$. Moreover, we consider functions $g \in L^2(\Sigma)$ and $y_0 \in L^2(\Omega)$ and controls $u \in L^2(Q)$ or $u \in L^2(\Sigma)$, depending on the underlying PDE.

Short formulations of the model problems with control u and state y then read

$$\min J_Q(y,u) \text{ subject to (2)} \qquad (P_Q)$$

and

$$\min J_\Sigma(y,u) \text{ subject to (4)}, \qquad (P_\Sigma)$$

respectively.

We now briefly summarize well-established results on existence and uniqueness of optimal solutions to Problems (P_Q) and (P_Σ), as well as first order necessary optimality conditions that are the basis for the Optimize then Discretize approach. We start with the solvability of the state equation. A known result by Wloka, [6], or Lions, [1] reads:

Theorem 1. *For any triple $(f,g,y_0) \in L^2(Q) \times L^2(\Sigma) \times L^2(\Omega)$ the initial-boundary value problem*

$$\begin{array}{rcll} y_t - \Delta y & = & f & \text{in } Q, \\ \partial_n y + \alpha y & = & g & \text{on } \Sigma, \\ y(t=0) & = & y_0 & \text{in } \Omega \end{array}$$

admits a unique solution

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

Here, $H^1(\Omega)^*$ denotes the dual space to $H^1(\Omega)$. Due to the fact that $U = L^2(Q)$ or $U = L^2(\Sigma)$, respectively, are not empty, the following theorem holds by standard arguments.

Theorem 2. *Under Assumption 1 and for J_Q and J_Σ defined in (1), (3) and arbitrary $\kappa > 0$, the optimal control problems defined in (P_Q) and (P_Σ) admit unique optimal controls $u^* \in U = L^2(Q)$ or $u^* \in U = L^2(\Sigma)$, respectively.*

Note that the associated optimal state y^* is uniquely determined by the optimal control u^* in either case by Theorem 1. In the following theorem we formulate the first order necessary optimality conditions for the control problems .

Theorem 3. *Let $u^* \in U = L^2(Q)$ be the optimal control of Problem (P_Q) and let y^* denote the associated optimal state. Then there exists an* adjoint state *$p \in W(0,T)$ as weak solution of*

$$\left.\begin{array}{rcll} -p_t - \Delta p & = & y^* - y_d & \text{in } Q \\ \partial_n p + \alpha p & = & 0 & \text{on } \Sigma \\ p(t=T) & = & 0 & \text{in } \Omega \end{array}\right\}, \qquad (5)$$

and the gradient equation

$$\kappa(u^* - u_d) + p \;=\; 0 \qquad (6)$$

is fulfilled for almost all $(x,t) \in Q$.

Analogously, let $u^* \in U = L^2(\Sigma)$ be the optimal control of (P_Σ) and let y^* denote the associated optimal state. Then there exists an adjoint state $p \in W(0,T)$ satisfying (5), and (6) is fulfilled for almost all $(x,t) \in \Sigma$.

For more details, we refer to [1] or [5].

We point out here that optimality conditions can not easily be formulated for all types of PDE-control problems. There is well-established theory available for linear-quadratic problems of the above types, as well as for some nonlinear problems of similar structure. Also, if additional bounds on the controls are given, well-known results can be applied. We refer for example to [1] for the treatment of these problems.

Another challenging problem are additional pointwise constraints on the state y. These types of problems have been subject to intensive research over the last years, and the theory is far from being complete. An attempt to handle certain state-constrained problems in COMSOL Multiphysics based on available theory has been undertaken in [4]. We refer to this paper and the references therein for further reading.

Theorem 3 reveals a typical feature of time-dependent optimal control problems: While the state equation (2) is an initial boundary value problem and hence a "forward-in-time" equation, the adjoint equation (5) runs backward in time. Even though (5) can by the time transformation $\tau = T - t$ be transformed into an initial-boundary-value problem

$$\left.\begin{array}{rcll} p_\tau - \Delta p & = & \tilde{y}^* - \tilde{y}_d & \text{in } Q \\ \partial_n p + \alpha p & = & 0 & \text{on } \Sigma \\ p(\tau=0) & = & 0 & \text{in } \Omega \end{array}\right\} \qquad (7)$$

where $\tilde{y}^*(x,\tau) = y^*(x,T-\tau)$, the reverse time directions for state and adjoint state remain a difficulty that needs to be taken into

account when solving such problems numerically.

A somewhat classical approach to deal with this problem is to sequentially solve the state and adjoint equation and to update the control in a gradient based optimization algorithm. We considered this strategy in [3], where our key objective has been to realize the reverse time directions without any low level data storage or copying.

A different solution approach and the focus of this paper is to treat the coupled optimality system in the whole space-time cylinder by interpreting the time variable as an additional space variable. We will explain this strategy and its implementation in COMSOL Multiphysics, conduct numerical experiments, and comment on the applicability as well as the limits of this approach.

2 Treating the Reverse Time directions by Simultaneous Space-Time Discretization

From the gradient equation (6), holding in the whole space-time domain Q or the boundary Σ depending on the type of problem, we obtain $u^* = u_d - \frac{1}{\kappa}p$, where u_d and p are evaluated in the whole domain or on the boundary, respectively. We insert this expression into the state equation (2) or (4). If the time variable t is treated as an additional space variable we obtain boundary-value problems of the form

$$\left.\begin{array}{rcl} y_t - \Delta y &=& u_d - \frac{1}{\kappa}p \\ -p_t - \Delta p &=& y - y_d \end{array}\right\} \text{ in } Q$$

$$\left.\begin{array}{rcl} \partial_n y + \alpha y &=& g \\ \partial_n p + \alpha p &=& 0 \end{array}\right\} \text{ on } \Sigma$$

$$\begin{array}{rcll} y &=& y_0 & \text{in } \Omega \times \{0\} \\ p &=& 0 & \text{in } \Omega \times \{T\}. \end{array}$$

for distributed control problems (P_Q), as well as

$$\left.\begin{array}{rcl} y_t - \Delta y &=& f \\ -p_t - \Delta p &=& y - y_d \end{array}\right\} \text{ in } Q$$

$$\left.\begin{array}{rcl} \partial_n y + \alpha y &=& u_d - \frac{1}{\kappa}p \\ \partial_n p + \alpha p &=& 0 \end{array}\right\} \text{ on } \Sigma$$

$$\begin{array}{rcll} y &=& y_0 & \text{in } \Omega \times \{0\} \\ p &=& 0 & \text{in } \Omega \times \{T\}. \end{array}$$

for boundary control problems (P_Σ), i.e. we consider Q to be a purely spatial domain of dimension $N+1$ with boundary $\Sigma \cup \Omega \times \{0\} \cup \Omega \times \{T\}$.

The algebraic systems coming up from this discretization can be solved by the implemented solvers of COMSOL Multiphysics without any further implementation effort, as we will see in the next section. Naturally, a main issue of this solution approach is the dimension of the discretized system. The fact that interpreting the time variable as additional space variable leads to an $(N+1)$-dimensional problem and limits the applicability of this strategy to problems in at most two space dimensions. On the other hand, this implementation strategy offers the opportunity of applying space-time adaptivity together. Yet, one has to be aware of the fact that by the above solution strategy a parabolic system is treated by elliptic solvers, which may induce instability issues. In a finite element discretization these may be overcome by discontinuous ansatz functions, as they are becoming an alternative in the optimal control community, cf. for instance [2].

3 Implementation and Numerical Examples

3.1 Distributed control

We consider first an example problem of form (P_Q) with distributed control where the data is given by $\Omega = (0,\pi)$, $T = \pi$, $\kappa = 0.01$, $\alpha = 0$, as well as $g = -\sin(t)$, and the desired functions

$$\begin{aligned} y_d(x,t) &= \sin(x)\,\sin(t) - \cos(x)(1+\pi-t), \\ u_d(x,t) &= \sin(x)(\sin(t)+\cos(t)) \\ &\qquad + \frac{1}{\kappa}\cos(x)(\pi - t). \end{aligned}$$

One can easily check that

$$\begin{array}{rcl} y^* &=& \sin(t)\sin(x). \\ u^* &=& \sin(t)\sin(x) + \cos(t)\sin(x), \\ p^* &=& -\kappa(u^* - u_d) \end{array}$$

solves the optimality system given in Theorem 3.

We assume that the reader is familiar with all steps involved in building the `fem`-struc-

ture for solving a single PDE and present some details of the COMSOL Multiphysics Script code that implements the described approach in the following. For the full code, we refer to [3].

First, we note that the time space domain $\Omega \times (0,T) = (0,\pi) \times (0,\pi)$ is defined as a two dimensional spatial domain with two "spatial" variables x and *time*:

```
fem.geom = rect2(0,pi,0,pi);
fem.sdim = {'x' 'time'}.
```

Assuming that all given data is defined in the usual way we introduce a global expression for the control u by

```
fem.globalexpr = {'u'...
        'ud(x,time)-p/kappa'};
```

Moreover, we obtain for the definition of the PDE and the boundary conditions:

```
fem.equ.ga = { { {'-yx' '0'};
             {'-px' '0'} } };
fem.equ.f  = { {'-ytime+u'...
     'ptime+y-yd(x,time)'} };
% boundaries: 1:t=0,2:x=pi,
%              3:t=pi,4:x=0
fem.bnd.ind = [1 2 3 2];
% boundary conditions:
fem.bnd.r  = { {'y-y0' 0};
               {0 0};
               {0 'p'} };
fem.bnd.g  = { {0 0};
               {'g(time)' '0'};
               {0 0} };
```

Once the definition of the problem is complete, the system can be solved by one of COMSOL Multiphysics' implemented solution routines. For the example above, we use the linear, nonadaptive elliptic solver `femlin`. We solve the problem on different grids, specified by the parameter `hmax`, using quadratic finite element functions. In the following table we show the L^2-errors $\|u^* - u_h\|_Q$ and $\|y^* - y_h\|_Q$ between the known optimal solution and the solution to the discretized problem (u_h, y_h) computed by COMSOL Multiphysics on the different grids. Figures 1–3 show the computed optimal control u_h, the computed optimal state y_h, as well as the associated adjoint state p_h.

h_{max}	$\|u^* - u_h\|_Q$	$\|y^* - y_h\|_Q$
2^{-2}	$1.6417 \cdot 10^{-2}$	$3.2837 \cdot 10^{-4}$
2^{-3}	$2.2293 \cdot 10^{-3}$	$3.0790 \cdot 10^{-5}$
2^{-4}	$3.0615 \cdot 10^{-4}$	$5.0814 \cdot 10^{-6}$
2^{-5}	$4.0305 \cdot 10^{-5}$	$4.9791 \cdot 10^{-7}$
2^{-6}	$5.3730 \cdot 10^{-6}$	$5.9155 \cdot 10^{-8}$

Tab. 1: Errors $\|u^* - u_h\|_Q$ and $\|y^* - y_h\|_Q$.

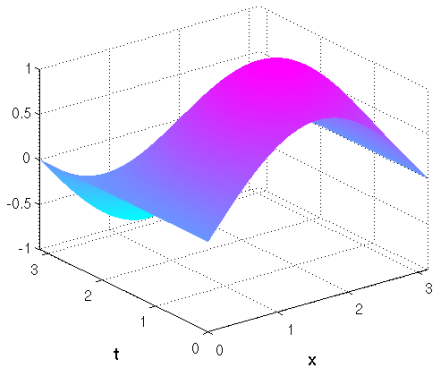

Fig. 1: optimal control u_h

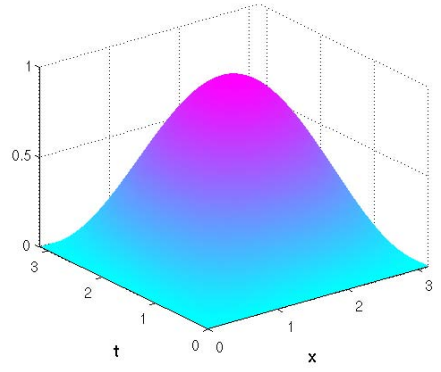

Fig. 2: optimal state y_h

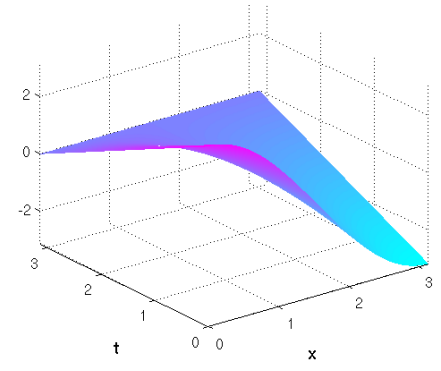

Fig. 3: adjoint state p_h

3.2 Boundary control

Now, we consider an example problem of form (P_Σ) with boundary control, very simi-

lar to the distributed control problem in the last section. The data is given by $\Omega = (0, \pi)$, $T = \pi$, $\kappa = 0.01$, $\alpha = 0$, as well as

$$\begin{aligned} f &= \sin(x)\cos(t) + \sin(x)\sin(t), \\ y_d &= \sin(x)\sin(t) - \cos(x)(1 + \pi - t), \\ u_d &= -\sin(t) + \frac{1}{\kappa}(\pi - t). \end{aligned}$$

One can easily check that

$$\begin{aligned} y^* &= \sin(t)\sin(x), \\ u^* &= -\sin(t), \\ p^* &= \cos(x)(\pi - t) \end{aligned}$$

solves the optimality system given in Theorem 3.

The implementation in COMSOL Multiphysics is very similar to the first example. We only need to substitute f for u as a source term of the state equation, as well as u for g, since u enters the state equation in the boundary conditions. This yields:

```
fem.equ.ga = { { {'-yx' '0'};
             {'-px' '0'} } };
fem.equ.f  = { {'-ytime+...
                 f(x,time)'...
     'ptime+y-yd(x,time)'} };
% boundaries: 1:t=0,2:x=pi,
%              3:t=pi,4:x=0
fem.bnd.ind = [1 2 3 2];
% boundary conditions:
fem.bnd.r  = { {'y-y0' 0};
               {0 0};
               {0 'p'} };
fem.bnd.g  = { {0 0};
               {'u' '0'};
               {0 0} };
```

Similar to the distributed example, we use the linear, nonadaptive elliptic solver `femlin` on different grids, specified by the parameter `hmax`. This time, we use linear finite element functions. The L^2-errors $\|u^* - u_h\|_\Sigma$ and $\|y^* - y_h\|_Q$ on the different grids are shown in Table 2. Figure 4 shows the computed optimal control u_h. The example has been constructed such that the optimal state y^* and the associated adjoint state p^* are the same as for the distributed control problem.

h_{max}	$\|u^* - u_h\|_Q$	$\|y^* - y_h\|_Q$
2^{-2}	$2.1379 \cdot 10^{-1}$	$2.5347 \cdot 10^{-2}$
2^{-3}	$1.0525 \cdot 10^{-1}$	$9.6450 \cdot 10^{-3}$
2^{-4}	$4.3199 \cdot 10^{-2}$	$2.9205 \cdot 10^{-3}$
2^{-5}	$1.7076 \cdot 10^{-2}$	$7.7394 \cdot 10^{-4}$
2^{-6}	$5.7762 \cdot 10^{-3}$	$1.9415 \cdot 10^{-4}$

Tab. 2: Errors for the boundary control problem.

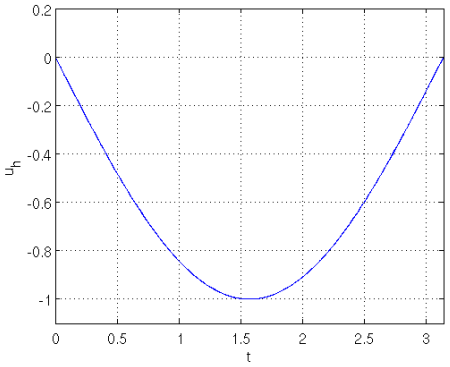

Fig. 4: Boundary control u_h

3.3 An example in 2D

In this example we use the 3D capability of COMSOL Multiphysics to solve a problem in two space dimensions. We consider the optimal control problem (P_Q) where the space-time domain is defined by $Q = (0, \pi)^2 \times (0, \pi) \subset \mathbb{R}^3$ and the functions y_d, u_d, and g are given by

$$\begin{aligned} y_d = \sin(x_1)\sin(x_2)\sin(t) \\ - \cos(x_1)\cos(x_2) \\ - 2\cos(x_1)\cos(x_2)(\pi - t), \end{aligned}$$

$$\begin{aligned} u_d = \sin(x_1)\sin(x_2)\cos(t) \\ + 2\sin(x_1)\sin(x_2)\sin(t) \\ + \frac{1}{\kappa}\cos(x_1)\cos(x_2)(\pi - t), \end{aligned}$$

$$g = -\vec{n}\sin(t)(\sin(x_1), \sin(x_2))^T,$$

respectively. The optimal solutions are

$$\begin{aligned} y^*(x_1, x_2, t) &= \sin(x_1)\sin(x_2)\sin(t) \\ u^*(x_1, x_2, t) &= \sin(x_1)\sin(x_2)(\cos(t) \\ &\qquad +2\sin(t)) \\ p^*(x_1, x_2, t) &= \cos(x_1)\cos(x_2)(\pi - t), \end{aligned}$$

which can easily be checked by inserting them into the optimality conditions of Theorem 3.

The differences in the implementation compared to the first example are only due to the higher space dimension of the problem. We define the 3D geometry by

```
% geometry and mesh:
  fem.geom = block3(pi,pi,pi,...
  'base','corner','pos',[0 0 0]);
```

and also account for the additional dimension in the definition of the PDE and the boundary conditions:

```
fem.equ.ga = { { {'-yx1' '-yx2' '0'}
                 {'-px1' '-px2' '0'}
               } };
fem.equ.f = { {'-ytime+u' 'ptime...
              +y-yd(x1,x2,time)'} };
fem.bnd.r = { {'y-y0' 0};
              {0 'p'};
              {0 0};
              {0 0} };
fem.bnd.g = { {0 0};
              {0 0};
              {'g1(x1,time)...
              -alpha*y' '-alpha*p'}
              {'g2(x2,time)...
             -alpha*y' '-alpha*p'}};
```

This time, we test the adaptive solver `adaption` with an initial grid determined by `hauto` and `ngen`, the number of new grid generations, set to two. In 3D, the space-time grid consists of tetrahedrons and the number of unknowns grows cubically when refining the grid. For that reason, we restrict our survey to three initial grids generated using `meshinit` where refinement is controlled by using the parameter `hauto` ranging from 7 to 5. We use again quadratic finite elements. In Figures 5–7 we present time-slice plots of u_h, y_h, and p_h.

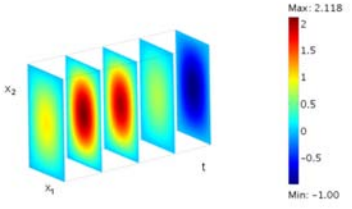

Fig. 5: u_h

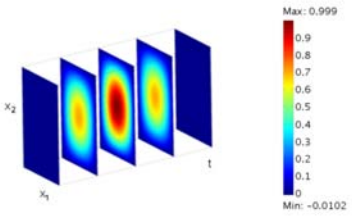

Fig. 6: y_h

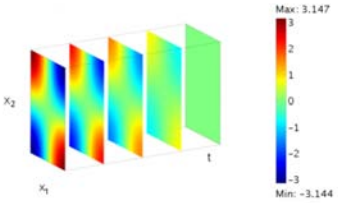

Fig. 7: p_h

hauto	$\|u^* - u_h\|_Q$	$\|y^* - y_h\|_Q$
7	$3.1710 \cdot 10^{-1}$	$4.7920 \cdot 10^{-3}$
6	$1.7107 \cdot 10^{-1}$	$2.3017 \cdot 10^{-3}$
5	$5.0385 \cdot 10^{-2}$	$5.4455 \cdot 10^{-4}$

Tab. 3: Errors to the 2D example, adaptive solver

4 Conclusion

We have successfully applied the finite element package COMSOL Multiphysics to simple time-dependent optimal control problems subject to PDE constraints by utilizing an Optimize then Discretize strategy.

The introduced strategy has proven to work reasonably well for our simple example problems. We take advantage of the fact that optimality conditions can be written in PDE form, which allows to apply a specialized PDE solver for optimization. The method we focused on is easily implementable and may well serve as a first step towards optimizing a given goal without the use of specialized optimization routines. The proposed approach does not substitute the use of specialized optimization software. One reason for that is that elliptic solvers are used for time-dependent parabolic control problems. This means in particular that the special role of the time is ignored, especially the fact that the time derivative of state and adjoint state is in general in a weak space $L^2(0,T,H^1(\Omega)^*)$, cf. Theorem 1. However, for cases with higher regularity our

approach seems more justified. In Figure 8, we show the error propagation through the space-time domain for the one-dimensional distributed control problem to illustrate this behavior due to solving a singular elliptic system.

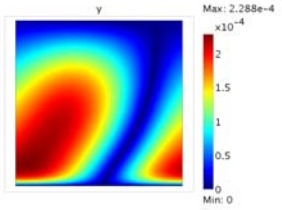

Fig. 8: Error flow through the space-time domain

The applicability of this strategy to other problems, even if optimality conditions can be formulated in PDE form, has to be decided on a case-to-case basis. Additional limitations are given by the size of the problem.

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The complete COMSOL Multiphysics-code of all examples is available on

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