Thomas Slawig[1] and Uwe Prüfert[2]
[1]Christian Albrechts Universiät zu Kiel and
[2]TU Bergakademie Freiberg

Mathematics-based Optimization in the COMSOL Multiphysics Framework

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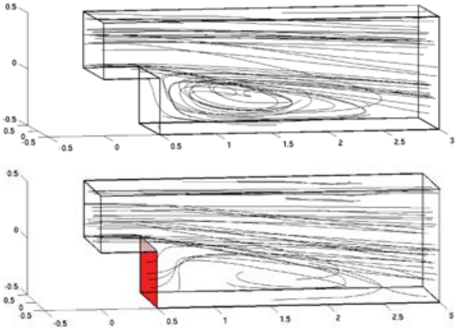
What is Optimal PDE Control? A Well Known Example

Control of the Navier-Stokes Equations, backward facing step.



Uncontrolled: A large vortex is located behind the step.

Controlled: The velocity on the vertical boundary (red colored) is used as **control**. The vortex is reduced.

Figures taken from:T. Slawig. *PDE-constrained Control using FEMLAB - Control of the Navier-Stokes Equations.*

Two General Appoches: First Discretize vs First Optimize

First discretize than optimize	First optimize than discretize
Discretize the whole problem by i.e. finite elements and use large scale optimizer to solve the problem.	Derive optimality conditions for the infinite dimensional problem. Here, this will be a system of coupled PDEs and algebraic equations in function spaces.
pro and contra	
- Discrete differential Operators fix the structure of the PDE (e.g. step sizes in space and time).	+ The structure of the problem as PDE system is conserved.
+ Optimality conditions are already known.	- Optimality conditions must be derived.
- Leads to huge discrete systems.	+ The effort depends on the used algorithms to solve the PDEs
+ One can use standard LP/NLP solvers.	+ Needs only an adequate PDE solver (like e.g. COMSOL Multiphysics).

Problem Definition

Let be $\Omega \subset \mathbb{R}^N$ a spatial domain with boundary Σ, (t_0, t_1) a time interval,

$$\min\ J_Q(y,u) := \frac{1}{2} \int_{t_0}^{t_1}\!\!\int_{\Omega} (y - y_d)^2 + \kappa(u - u_d)^2 \ dx\, dt$$

subject to

$$\begin{array}{rcll} \frac{d}{dt}y - \nabla \cdot (A\,\nabla y) + a_0 y & = & u & \text{in} \quad Q := \Omega \times (t_0, t_1), \\ \vec{n} \cdot (A \nabla y) + \alpha y & = & g & \text{on} \quad \Sigma, \\ y & = & y_0 & \text{in} \quad \Omega_0 := \Omega \times \{0\} \end{array} \qquad (1)$$

and the control constraints (optional)

$$\underline{u} \le u \le \overline{u} \quad \text{in} \quad Q$$

for given functions $\underline{u}$, $\overline{u}$, y_d, and u_d. A and $a_0 \in L^\infty(\Omega)$. In the following we refer this setting by (P). The function u is the **control** and y is the **state**.

Existence and Uniqueness

By a simple transformation, one can bring (1) into a homogeneous form, i.e. $g = 0$, $y_0 = 0$, etc. but with an additional source term f.

Theorem

Assume that Ω is a bounded domain with sufficiently smooth boundary Γ. If the data y_0 , g and the control u are sufficiently smooth, then the weak solution y of the initial value problem (2.1) belongs to

$$H^{2,1}(Q) = L^2(t_0, t_1; H^1(\Omega)) \cap H^1(t_0, t_1; L^2(\Omega)).$$

The weak formulation can be written as

$$\int_\Omega \frac{d}{dt} yw\,dxdt + \int_\Omega (A\nabla y)\cdot\nabla w\,dxdt + a_0 \int_\Omega yw\,dxdt = \int_\Omega (u+f)w\,dxdt \quad \forall w \in H^{1,0}(Q),$$

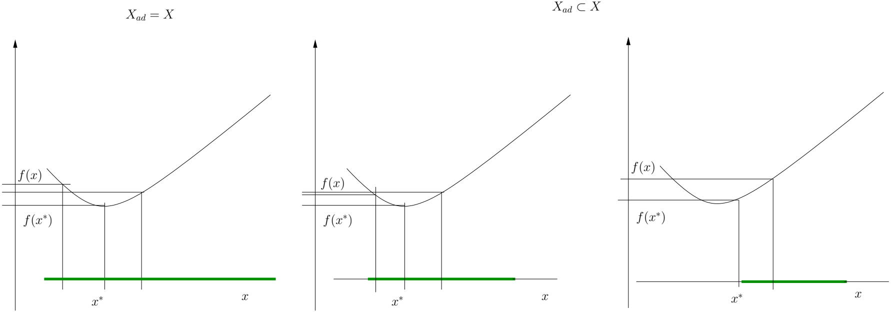
$$y(x, t_0) = 0 \quad \textit{in } \Omega.$$

Note:

- That is a surprisingly regular function space.
- As we will see later, the control u will be sufficiently smooth in our case.

Optimality Conditions: The real valued case

Assume that $f(x)$ is a strongly convex differentiable function on X_{ad}. We consider the problem $\min f(x)$ on $X_{ad} \subseteq X$.



- Optimality condition: $\frac{d}{dx} f(x^*)(x - x^*) \geq 0$ for all $x \in X_{ad}$ where X_{ad} is the admissible (subset) of the control space X.
- If $X_{ad} = X$ (i.e. the problem is unconstrained) we have $\frac{d}{dx} f(x^*) = 0$ is already sufficient for optimality.

Optimality Conditions: PDE Case

Theorem

A control u^* is the optimal solution of (P) if and only if, together with the associated optimal state y^* and the adjoint state p, it solves the system

$$\left.\begin{array}{rcl} \frac{d}{dt}y^* - \nabla\cdot A\nabla y^* + c_0 y^* &=& u^* + f \\ -\frac{d}{dt}p - \nabla\cdot A\nabla p + c_0 p &=& y^* \end{array}\right\} \quad \text{in } Q$$

$$\left.\begin{array}{rcl} \vec{n}\cdot(A\nabla y^*) &=& 0 \\ \vec{n}\cdot(A\nabla p) &=& 0 \end{array}\right\} \quad \text{on } \Sigma$$

$$y^*(t_0) = 0 \quad \text{in } \Omega$$

$$p(t_1) = 0 \quad \text{in } \Omega$$

and

$$u^* \in U_{ad} := \{u \in L^2(Q) : \underline{u} \le u \le \bar{u} \ \text{ a.e. in } Q\}, \tag{2}$$

$$(\kappa u^* + p, u - u^*) \ge 0 \text{ for all } u \in U_{ad}(Q). \tag{3}$$

As in the real valued problem, the last two conditions can be replaced by $\kappa u^* + p = 0$ if $U_{ad} = L^2(Q)$.

Implementing the PDE part of the problem in COMSOL Multiphysics is strait forward, but how we can deal with the inequality condition?

Inequality Condition in Terms of Projection

- One can show that (2)–(3) is equivalent to $u^* = \min\{\overline{u}, \max(\underline{u}, -\frac{1}{\kappa}p)\}$.
- For functions $a, b, z \in L^\infty(Q)$ we define the point wise projection

$$\Pi_{[a,b]}\{z\} := \pi_{[a(x,t),b(x,t)]}\{z(x,t)\}\, \forall (x,t) \in Q,$$

  where $\pi_{[a,b]}\{z\} := \min\{b, \max(a,z)\}$, $a, b, z \in \mathbb{R}$.
- Using

$$\max(a,b) = \frac{1}{2}(a + b + \mathsf{sign}(a-b)(a-b))$$
$$\min(a,b) = \frac{1}{2}(a + b - \mathsf{sign}(a-b)(a-b)),$$

  by using a smooth implementation of the signum function by – e.g. COMSOL's `flsmsign` -- we obtain a smooth projection formula.
- Now we can replace (2)–(3) by a smooth projection $u^* = \tilde{\mathbb{P}}_{[\underline{u},\overline{u}]}\left\{-\frac{1}{\kappa}p\right\}$.

The Optimality System to Solve by COMSOL

PDE System

Consequently, we obtain a **smooth** system of PDEs we can easily solve by COMSOL Multiphysics

$$\left.\begin{array}{rcl} \frac{d}{dt}y^* - \nabla\cdot A\nabla y^* + c_0 y^* &=& \tilde{\mathbb{P}}_{[\underline{u},\overline{u}]}\left\{-\frac{1}{\kappa}p\right\} + f \\ -\frac{d}{dt}p - \nabla\cdot A\nabla p + c_0 p &=& y^* \end{array}\right\} \quad \text{in } Q$$

$$\left.\begin{array}{rcl} \vec{n}\cdot(A\nabla y^*) &=& 0 \\ \vec{n}\cdot(A\nabla p) &=& 0 \end{array}\right\} \quad \text{on } \Sigma$$

$$y^*(t_0) = 0 \quad \text{in } \Omega$$

$$p(t_1) = 0 \quad \text{in } \Omega.$$

- Only two unknowns, control u implicitly given.
- Discretize the time-space domain by a triangular mesh.
- Unfortunately, this restricts this approach to a space dimension up to two (for time dependent problems).

Numerical Example

- Solve Problem (P) with $A = \mathbb{I}$ and $-1 \leq u \leq 1.5$ in $Q = (0, \pi) \times (0, \pi)$, $y_d = \sin(x)\sin(t)$ and $u_d \equiv 0$. $\kappa = 10^{-3}$.
- Use weak form to implement the PDE system, mesh Q by a **space-time grid** via

  ```
  fem.geom = rect2(0,pi,0,pi);
  ```

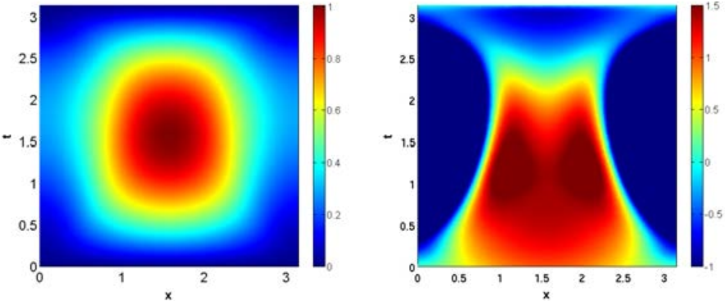
  The PDE reads as

  ```
  fem.equ.ga = { { {'-yx' '0'}
                   {'-px' '0'} } };
  fem.equ.f  = { {'-ytime+min(u_b,max(u_a,1/kappa*p))' ...
                 ' ptime+y-y_d'} };
  ```
- Replace `max` by a smooth projection using `flsmsign` with explicitly given regularization parameter ϵ.

Note: This example **only illustrates** the approach, for more realistic problems see e.g. Ira Neitzel, Uwe Prüfert, and Thomas Slawig. *Solving Time-Dependent Optimal Control Problems in COMSOL Multiphysics.*

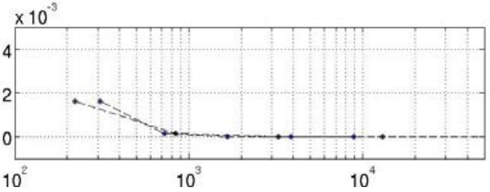
Results I

Problem solved by COMSOL Multiphysics. We run the program for various grids, both uniformly and adaptively refined. The optimal control is boxed between $\underline{u} = -1$ and $\overline{u} = 1.5$.

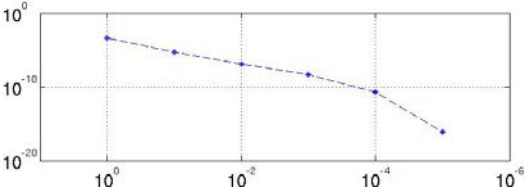


Left: Computed optimal state y
Right: computed optimal control $u = \min(1.5, \max(-1, 1000 \cdot p))$

Results II



Values of $\frac{1}{J(y,u)}|J(y,u) - \overline{J(y,u)}|$ over number of grid points. Black uniformly, blue adaptively refined mesh. $\overline{J(y,u)}$ is the solution on the finest mesh.



Values of $\frac{\|y^\epsilon - \overline{y}\|}{\|\overline{y}\|}$ over the regularization parameter for `flsmsign`. $\overline{y}$ is a reference solution computed by COMSOLs choice of smoothing parameter.

Conclusion and Remarks

- If optimality conditions in terms of PDE are available, COMSOL can be used to solve optimal control problems with control constraints.
- We have to re-write the Optimal Control Problem to fit it in the COMSOL framework.
- The handling of the Variational Inequality (3) by a smoothed projection within COMSOL can be justified.
- The approach is not restricted to our problem class, c.f.
  - Navier-Stokes Equations: T. Slawig. *PDE-constrained Control using FEMLAB - Control of the Navier-Stokes Equations. Numerical Algorithms,* **42** (2), *pp. 107–126*, 2006
  - Burger's equation: F. Yilmaz and B. Karasözen. *Solving Distributed Optimal Control Problems for the Unsteady Burgers Equation in COMSOL Multiphysics*. Journal of Computational and Applied Mathematics, **235**, *(16)* pp. 4839–4850, 2011

Acknowledgments

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