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Mathematics-based Optimization in the Comsol Multiphysics Framework

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Abstract: We show how the equation-based modeling feature in Comsol Multiphysics can be used to perform mathematics-based optimization. We show how mathematics can be used to determine conditions for optima of problems that are described and solved by Comsol Multiphysics. The approach that we present here is to derive an equation-based model for gradients or sensitivities for the considered application, and use Comsol Multiphysics again to compute them. This method has been used in an abstract setting in the mathematical optimal control and optimization community for several example problems and application ranging from heat equation to fluid mechanical problems described by the Navier-Stokes equations. We give an impression how the method can be used and how efficient it can be. Moreover we show are non-differentiable control-constrained problems can be smoothed to apply Comsol Multiphysics's built-in Newton solver.

1 Introduction

Simulations now play an important role in scientific and engineering sciences, since they allow for faster and cheaper prototyping compared, e.g., to experiments. However, in many applications the overall goal is not just to simulate a given process or problem, but to obtain an optimal solution, optimal parameters or an optimal design or geometry.

While the engineer's and scientist's knowledge is crucial at this point, still numerical algorithms can be a helpful tool in optimization or design, too. There are many algorithms suitable and applicable when optimizing an already discretized formulation of a scientific problem. Since those problems are mostly given as partial differential equations (PDEs), their discrete counterparts can be formulated and solved by modern simulation software. One example for such kind of software is Comsol Multiphysics®, which is based on the finite element method and solves the generated discrete systems by a variant of Newton's method (in the interesting and most challenging nonlinear case). Comsol Multiphysics even supplies an optimization routine which can be used to perform the above mentioned optimization tasks for finitely many real-valued parameters representing material coefficients, initial or boundary values or the model geometry, depending on the desired optimization parameter. This process of first discretizing the problem (e.g. by the finite element method) and then solving an optimization problem with finitely many parameters is sometimes called the *first-discretize-then-optimize* approach.

On the other hand, in the mathematical community of optimal control methods are developed study optimization problems in a very abstract mathematical setting in function spaces, see among others [7, 9, 15] for an overview. As for real-valued functions, then conditions (comparable to the well-known conditions $f'(x) = 0$ or $\operatorname{grad} f(x) = 0$) that characterize optimal solutions are stated and proved. These conditions are called optimality systems and are PDEs again. The contains the original equation (which is then called state equation) and a second equation called adjoint equation for a second quantity, the so-called *adjoint state*. With the help of the adjoint state the optimal control or parameters can be characterized.

Since the optimality system is a PDE (system) again, it can be afterwards discretized and solved by appropriate software, and consequently Comsol Multiphysics can be used to apply the finite element method again. Following this approach is sometimes called *first optimize then discretize*.

In this paper we want to give an example for this approach using Comsol Multiphysics. We study an parabolic control problem with additional bound constraints on the parameters.

For parabolic, i.e., time-dependent PDEs, the optimality system contains a forward and a backward-in-time equation which are coupled by an algebraic equation. To solve this system, iterative algorithms are in use. Another approach is to solve both equations at once, i.e. as a huge system of coupled equations, cf. for example [12]. This approach is also used here. that means the optimality system is solved as one system of elliptic PDEs including the use of (optionally adaptive) space-time meshes. The method is justified by an equivalence result stated in [11], where also detailed proofs of the underlying mathematical theory can be found.

Problems with bound or box constraints on the control variables or parameters are mathematically challenging, since in this case the resulting optimality system becomes non-differentiable. More precise, a non-differentiable projection operator additionally occurs in the coupling equation between adjoint state and control. The resulting non-smooth system can be solved e.g. by semi-smooth Newton methods, cf. for example [5, 7, 8]. Moreover, beginning in the late 1990s, the concept of smoothing functions was studied in various papers, see e.g. [2]. Here we show how a so-called regularized, i.e. smoothed formulation of the optimality system can be obtained and solved. Here we some additional features of COMSOL MULTIPHYSICS that provides e.g. a smoothed signumfunction. The idea for this regularization came from a formal transformation of the optimality system of the (constrained or unconstrained) control problems: Treating both space and time similarly, it becomes a biharmonic boundary value problem whose weak form involves an elliptic bilinear form. This method was also used in [1] and is described in detail in [11]. The transformation involves expressing the control by the adjoint state, as in [6]. Biharmonic equations (with respect only to spatial variables) are well-known from elasticity problems and can be solved by e. g. finite elements, see e. g. [4, 13].

COMSOL MULTIPHYSICS allows to write the non-differentiable projection formula occurring in constrained problems symbolically as a combination of minimum and maximum functions. These terms and the whole PDE are differentiated symbolically rather than numerically when nonlinear solvers are applied. Moreover the smoothed, regularized projection formula presented here can also easily be implemented using built-in functions. We point out the work in [10], where we focused on the implementation issues of the proposed approach.

This paper is organized as follows: After the introduction into the problem class in Section 2, we briefly state the known results of existence and uniqueness of the equations that are crucial for a mathematical analysis. Then we state the optimality system for unconstrained and constrained problems and show how a smoothed version can be obtained. We discuss the justification of this approach by stating a convergence result. Finally we present a numerical example illustrating our approach.

2 Problem formulation

In this section we present a model example which is used to illustrate our approach. It is a typical distributed optimization or control problem for a linear time-dependent parabolic PDE.

Let Ω be a bounded subset of $\mathbb{R}^N$ $(N = 1, 2)$ with smooth boundary Γ, and let the time interval be given as $[0, T]$.

We consider the optimal control problem (P) with a tracking type objective functional

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

subject to the PDE (state equation) in weak form, with distributed control u,

$$\left.\begin{array}{rcll} y_t - \Delta y + c_0 y &=& u & \text{in } Q := \Omega \times (0,T) \\ \vec{n} \cdot \nabla y &=& g & \text{on } \Sigma := \Gamma \times (0,T) \\ y(x,0) &=& y_0 & \text{on } \Omega. \end{array}\right\} \quad (2.1)$$

Here y_d, u_d, c_0, y_0, g are given data, $\kappa > 0$ is a regularization parameter, and $\vec{n} \cdot \nabla y$ stands for the outward normal derivative of y. The necessary assumptions on the data will be given later on. To simplify the theory, let $c_0 > 0$ be a real number.

Moreover we will consider a second control problem (P_{con}) where additional control constraints of linear type,

$$u_a(x,t) \leq u(x,t) \leq u_b(x,t) \quad \text{in } Q \qquad (2.2)$$

with $u_a(x,t) < u_b(x,t)$ in Q, are imposed.

3 Existence and uniqueness of weak solutions

Since COMSOL MULTIPHYSICS uses discretized weak formulations in the Finite Element method, we now recall those for our model problem. These are obtained by multiplying the PDE by test functions (denoted below by w), integrating over the domain (in our case the space-rime domain Q), and then optionally perform an integration by parts. The resulting integral equations can be solved under weaker differentiability assumptions. In this subsection we briefly summarize the known results on existence, uniqueness and regularity of the PDE. This rigorous analysis is the basis of our mathematical characterization of solutions to the control problem and thus also for our solution approach based on equation-based modeling in COMSOL MULTIPHYSICS.

Just for this analysis, the problem above is equivalently transformed to a homogeneous one by setting $\tilde{y} := y - y_d, \tilde{u} := u - u_d$ and considering

$$\min \tilde{J}(\tilde{y},\tilde{u}) = \frac{1}{2}\int_Q \tilde{y}^2 + \kappa\tilde{u}^2 \, dxdt.$$

Additionally, the right-hand side of the equation will be modified. Since this directly enters the weak from we give the resulting transformed function $\tilde{f}$ (that replaces f) below. Also the optional control constraints in (P_{con}) are replaced by

$$\tilde{u}_a \quad \leq \; u \; \leq \quad \tilde{u}_b \quad \text{a.e. in } Q \qquad (3.1)$$

for $\tilde{u}_a := u_a - u_d, \tilde{u}_b := u_b - u_d$.

The following theorem provides the unique weak solvability of the state equation, and also higher regularity of the solution. Note that we omit the tildes here for simplicity, i.e., y refers to y etc.

Theorem 3.1. *Assume that $\Omega \subset \mathbb{R}^N$ is a bounded domain with sufficiently smooth boundary Γ. If the data y_0, g and the control and ua re sufficiently smooth, then the weak solution y of the initial value problem* (2.1) *belongs to*

$$H^{2,1}(Q) = L^2(0,T;H^1(\Omega)) \cap H^1(0,T,L^2(\Omega)).$$

The weak formulation of the problem can be written as

$$\int_Q y_t w\,dxdt + \int_Q \nabla y\cdot\nabla w\,dxdt + c_0\int_Q yw\,dxdt$$
$$= \int_Q (u+f)w\,dxdt \quad \forall w\in H^{1,0}(Q), \qquad (3.2)$$
$$y(x,0)=0 \text{ in } \Omega.$$

Proof. See [15, Theorems 3.9, 3.12, 3.13, Lemma 7.12], and [3], where this has been proven for a problem with homogeneous Dirichlet boundary conditions. The proof can be adapted to problems with homogeneous Neumann boundary conditions, for more details see [11]. □

4 Characterization of Optimal Solutions

In this section we state the existence and uniqueness of solutions to the control problems (P) and (P_{con}), respectively, and present the so-called *Optimality Systems*, i.e., characterizations of these optimal solutions. For more detailed information, we refer for example to [14]. We begin with the existence and uniqueness result.

Theorem 4.1. *For all $\kappa > 0$, problems (P) and (P_{con}) have unique solutions in $L^2(Q)$, here both denoted by u^*.*

Proof. The proof is given in [15, Thm. 3.15]. □

The optimality systems that characterize the unique optimal solutions are the counterparts of the well-known condition $f'(x)=0$ or $\text{grad} f(x)=0$ for optima of a real-valued function f. They are summarized in the following subsections.

Unconstrained Problem

We begin with the unconstrained problem. Note that they are both necessary and sufficient for optimality by the convexity of J.

Theorem 4.2. *A control u^* is the optimal solution of (P) if and only if the triple (y^*, p, u^*) with state y^* and adjoint state p is a weak solution of the system*

$$\left.\begin{aligned} y_t^* - \Delta y^* + c_0 y^* &= u^* + f \\ -p_t - \Delta p + c_0 p &= y^* \end{aligned}\right\} \text{ in } Q \quad (4.1)$$
$$\left.\begin{aligned} \vec{n}\cdot\nabla y^* &= 0 \\ \vec{n}\cdot\nabla p &= 0 \end{aligned}\right\} \text{ on } \Sigma \quad (4.2)$$
$$y^*(x,0) = 0 \quad \text{in } \Omega \quad (4.3)$$
$$p(x,T) = 0 \quad \text{in } \Omega \quad (4.4)$$
$$\kappa u^* + p = 0 \quad \text{in } Q. \quad (4.5)$$

Here we call (y^*, p, u^*) a weak solution if it satisfies (3.2),(4.5), and

$$-\int_Q p_t w\,dxdt + \int_Q \nabla p\cdot\nabla w\,dxdt + c_0\int_Q pw\,dxdt$$
$$= \int_Q y^* w\,dxdt \quad \forall w\in H^{1,0}(Q), \qquad (4.6)$$
$$p(x,T)=0 \quad \text{in } \Omega.$$

The adjoint state p is uniquely determined.

Proof. See [15, Lemma 3.17 and Theorem 3.21]. □

The PDE for p is called adjoint equation, and (4.5) is often referred to as the gradient equation. It can be used to eliminate the control in the state equation by setting $u^* = -\frac{1}{\kappa}p$.

Constrained Problem

For the constrained problem (P_{con}) we obtain the following result.

Theorem 4.3. *A control $u^*\in L^2(Q)$ is the optimal solution of (P_{con}) if and only if the triple (y^*, p, u^*) with the state y^* and the adjoint state p is a weak solution of the same system as in Theorem 4.2 with (4.5) replaced by*

$$u^*\in U_{ad} := \{u\in L^2(Q) : u_a\le u\le u_b \text{ in } Q\},$$
$$\int_Q (\kappa u^* + p)(u-u^*)dxdt \ \ge\ 0 \quad \forall u\in U_{ad}. \quad (4.7)$$

Proof. See [15, Theorem 3.21]. □

Note that in this case u^* cannot be replaced by the adjoint state p in a simple way. Instead, projection formulas are in use, which we will explain now.

Optimality conditions in terms of projections

We consider now the homogenized version of the control constrained problem (P_{con}) and replace the variational inequality (4.7) by the projection formula

$$u^* = \mathbb{P}_{[u_a,u_b]}\left\{-\frac{1}{\kappa}p\right\}, \qquad (4.8)$$

where for functions $a, b, z : Q\to\mathbb{R}$ we have used the point-wise projection

$$\mathbb{P}_{[a,b]}\{z\} := \pi_{[a(x,t),b(x,t)]}\{z(x,t)\},\ (x,t)\in Q, \ (4.9)$$

with

$$\pi_{[a,b]}\{z\} := \min\{b, \max(a,z)\}, \quad a,b,z\in\mathbb{R}. \ (4.10)$$

Then, we can write the optimality conditions for the constrained problem as (4.1)–(4.4), together with (4.8) which replaces (4.5), all in weak sense.

A Regularized Projection Formula

In order to avoid the non-differentiable term due to the min and max function in the projection formula, we replace the latter by a smoothed one. Since we may write for $a, b \in \mathbb{R}$

$$\begin{aligned} \max(a,b) &= \frac{a+b+\operatorname{sign}(a-b)\cdot(a-b)}{2}, \\ \min(a,b) &= \frac{a+b-\operatorname{sign}(a-b)\cdot(a-b)}{2} \end{aligned}$$

the signum function is the source of non-differentiability of the max / min functions, a way around this problem is to replace sign by a smooth approximation. This is for example the function `flsmsign` used in COMSOL MULTIPHYSICS.

For our theoretic results below we define for $\varepsilon > 0$ the smoothed sign-function smsign by

$$\operatorname{smsign}(z;\varepsilon) := \begin{cases} -1 & z < -\varepsilon \\ \mathcal{P}(z) & z \in [-\varepsilon, \varepsilon]\,, \\ 1 & z > \varepsilon \end{cases} \tag{4.11}$$

where $\mathcal{P}$ is a polynomial of seventh degree that fulfills

$$\begin{aligned} \mathcal{P}(\varepsilon) = 1, \mathcal{P}(-\varepsilon) = -1, \mathcal{P}^{(k)}(\pm\varepsilon) &= 0,\ k = 1,2, \\ \int_0^{\varepsilon} \mathcal{P}(z)dz = -\int_{-\varepsilon}^{0} \mathcal{P}(z)dz &= \varepsilon. \end{aligned}$$

This polynomial is explicitly given in [11]. The only difference to `flsmsign` is that the latter is defined as piecewise polynomial of seventh degree, whereas we define `smsign` as polynomial on $(-\varepsilon, \varepsilon)$). This difference between `flsmsign` and `smsign` will not change the theory.

For the smoothed signum function defined above, we can prove (see [11] for details) the following convergence results for $\varepsilon \to 0$.

Lemma 4.4. The smoothed sign-function defined in (4.11) converges point-wise towards sign:

$$\operatorname{smsign}(z;\varepsilon) \overset{\varepsilon\to 0}{\longrightarrow} \operatorname{sign}(z) \quad \forall z \in \mathbb{R}$$

and in all L^q-norms with $1 \le q < \infty$, i.e.,

$$\lim_{\varepsilon\to 0}\left(\int_{\mathbb{R}} |\operatorname{smsign}(z,\varepsilon) - \operatorname{sign}(z)|^q dz\right)^{1/q} = 0.$$

Based on the smoothed signum function, we can now for arbitrary $\varepsilon > 0$ define smoothed $\max^{(\varepsilon)}, \min^{(\varepsilon)}$ functions (replacing the signum function by smsign with parameter ε). Furthermore, we replace the projections π and $\mathbb{P}$ defined in (4.10) and (4.9) by their corresponding smoothed counterparts $\pi^{(\varepsilon)}$ and $\mathbb{P}^{(\varepsilon)}$. Since we want to use the projection $\mathbb{P}^{(\varepsilon)}$ in the optimality system, we prove in [11] the following convergence result.

Theorem 4.5. *Let $a, b \in L^\infty(Q)$ be given functions. The smoothed projection $\mathbb{P}^{(\varepsilon)}_{[a,b]}$ converges towards $\mathbb{P}_{[a,b]}$ in all L^p-norms with $1 \le p < \infty$ as $\varepsilon \to 0$.*

Moreover, in [11] it is shown that the solution to the regularized problem (i.e., the one where the projection $\mathbb{P}$ is replaced by its smoothed counterpart $\pi^{(\varepsilon)}$), converges to the solution of the unregularized one, i.e., original problem.

Theorem 4.6. *For $\varepsilon \to 0$ the corresponding sequence of regularized optimal controls $\{u^\varepsilon\}$, where*

$$u^\varepsilon := \mathbb{P}^{(\varepsilon)}_{[u_a,u_b]}\left\{-\frac{1}{\kappa}p^\varepsilon\right\}$$

and p^ε denotes the adjoint state of the regularized problem, converges to u^*.

This result justifies the use of the smoothed version of the problem. Concluding, we point out that the proposed regularization avoids the presence of non-differentiable terms in the optimality system associated with optimal control problems with bounds on the control. The regularized problems admit unique solutions that converge to the unregularized ones for vanishing regularization parameters.

5 Numerical experiments

As example we consider

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

while (y, u) fulfills the parabolic PDE

$$\begin{aligned} y_t(x,t) - \Delta y(x,t) &= u(x,t) && \text{in } Q \\ \vec{n}\cdot\nabla y(x,t) &= 0 && \text{on } \Sigma \\ y(x,0) &= 0 && \text{on } \Omega. \end{aligned}$$

and the constraints on the control $-1 \le u \le 1.5$ in $Q = (0,\pi)\times(0,\pi)$. The desired state is given by $y_d = \sin(x)\sin(t)$ and the control shift u_d vanishes identically. We set $\kappa = 10^{-3}$. The optimal solution of this problem is unknown.

The presence of nontrivial data y_d, u_d, y_0, and g slightly changes the optimality systems previously derived in Section 2 when considering the inhomogeneous problem formulation for the theoretical results. Details are given in [11]. we do not mention hem here; we only want to show that our approach is working.

For our computations, we choose COMSOL MULTIPHYSICS, where we are mainly interested in using some of the programs build-in tools like adaptivity and multigrid solvers. We computed the solutions on a space-time-mesh. COMSOL MULTIPHYSICS does provide a smoothed signum function `flsmsign` that is very similar to our choice. Note again that the only difference is that in the specification of `flsmsign` it is defined as piecewise polynomial of seventh degree, whereas we define `smsign` as polynomial on $(-\varepsilon, \varepsilon)$). Once again we state that this difference does not affect our mathematical theory sketched above.

COMSOL MULTIPHYSICS by default uses the smoothed min/max functions but without user-control of the smoothing parameter ε. In our computations we use our smoothed projection formula and therein `flsmsign`, where the parameter ε remains in the hands of the user. For details on the implementation of optimality systems in COMSOL Multiphysics we refer to [10]. Note, however, that the described approach is not limited to special software.

Uniformly Refined Meshes

We solve the example first by the `femnlin` solver on uniformly refined meshes, starting from the coarsest one in COMSOL MULTIPHYSICS. The smoothing parameter was $\varepsilon = 10^{-4}$.

From Table 1 we observe that the solution process converges for all meshes. The number of Newton iterations seems to be mesh nearly independent, and convergence of state and control with respect to the grid size h can be seen.

	#pts	#it	$\|y_h - y_d\|$	$\|u_h\|$	$J(y, u)$
0	61	7	0.18416	2.9992	0.021456
1	221	8	0.18152	3.0184	0.02103
2	841	8	0.18128	3.0223	0.020999
3	3281	8	0.18124	3.0238	0.020996
4	12961	8	0.18123	3.0243	0.020996
5	51521	12	0.18123	3.0244	0.020996

Table 1: Results for uniformly refined mesh. First column is the number of refinements, second the number of grid points, and third the number of needed iterations to converge.

Adaptively Refined mesh

Here we use the adaptive solver on the initial mesh of the computation above. We control the number of new grids created by the error controller of the adaptive solver. The values state, control and cost function in Table 2 are comparable with the results above for the uniformly refined mesh.

	#pts	#it	$\|y_h - y_d\|$	$\|u_h\|$	$J(y_h, u_h)$
1	139	13	0.1818	3.0115	0.02106
2	311	15	0.18147	3.0185	0.021021
3	725	16	0.1813	3.0218	0.021001
4	1661	17	0.18126	3.0232	0.020997
5	3867	18	0.18124	3.0240	0.020996
6	8884	19	0.18124	3.0242	0.020996

Table 2: Adaptively refined mesh. First column is the number of generation in the adaptive refinement process, second and third column as above.

Convergence of the Smoothed Solutions

Having the convergence proof for the regularized problems, we compare solutions computed by the regularized projection with solutions computed by COMSOL MULTIPHYSICS's built-in min/max functions.

Table 3 numerically shows the convergence of state, control and adjoint state while the regularization parameter ε going to zero. Figure 1 visualizes the values presented in Table 3 and shows the convergence with respect to ε.

ε	$\frac{\|y_\varepsilon - y^*\|}{\|y^*\|}$	$\frac{\|u_\varepsilon - u^*\|}{\|u^*\|}$	$\frac{\|p_\varepsilon - p^*\|}{\|p^*\|}$
1e-0	4.4400e-04	1.6626e-02	2.9988e-03
1e-1	5.5765e-06	1.1005e-04	1.8942e-05
1e-2	1.1685e-07	1.3176e-06	3.5138e-07
1e-3	4.1875e-09	6.8397e-08	1.2940e-08
1e-4	1.8675e-11	2.3611e-10	6.9580e-11
1e-5	6.9621e-17	4.1289e-16	3.2053e-16

Table 3: Relative error between the solutions computed by the regularized projection formula (indicated by ε) and COMSOL MULTIPHYSICS's min/max functions (indicated by an asterix).

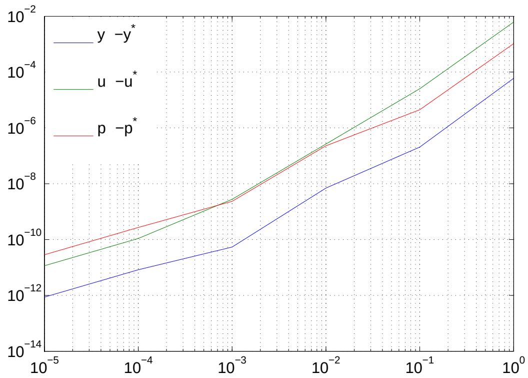

Figure 1: Relative difference between the solutions computed by the regularized projection formula. Both axis are scaled logarithmically.

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