Optimal PDE Control Using COMSOL Multiphysics

Ira Neitzel, Uwe Prüfert, and Thomas Slawig

This optimal control problem is a sub-topic of project A1 within MATHEON*.

Problem Setting

Regional hyperthermia is a cancer therapy aiming at heating large, deeply seated tumors in order to make them more susceptible to an accompanying radio or chemo therapy. The heat is introduced into the human body by absorption of radio-frequency electromagnetic waves originating from a phased array applicator.

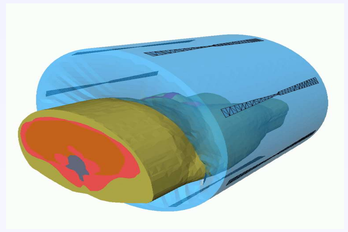

Figure 1: Virtual patient in a microwave applicator. Picture courtesy of Zuse Institute Berlin.

The aim of optimal control of the hyperthermia problem is:

- The tumor should be heated up to the therapeutic temperature.
- The temperature in the healthy tissue should not be higher than a compatible temperature.

The temperature distribution is driven by the bio-heat-transfer equation (BHTE), which is of elliptic type.

We consider the optimal control problem (HYPER):

$$\min \frac{1}{2}\int_\Omega (T-T_d)^2 + \kappa u^2 dx$$

subject to the elliptic PDE

$$\begin{aligned} -\nabla\cdot(A\nabla T) + a_0(T-T_{37}) &= u \text{ in } \Omega \\ \vec{n}\cdot(A\nabla T) + \alpha_0(T-T_b) &= 0 \text{ on } \Gamma. \end{aligned} \tag{1}$$

Further we have the constraints on the temperature:

$$\begin{aligned} T_{therapeutic} \;\leq\; T \quad &\text{in } \Omega_{tumor} \\ T \leq T_{healthy} &\text{ in } \Omega\backslash\Omega_{tumor}\,. \end{aligned}$$

Theoretical Preparations

We introduce a barrier functional by e.g.

$$\begin{aligned} b(T;\mu) = -\mu\int_\Omega &\ln(T-T_{therapeutic}) \\ &+ \ln(T_{healty}-T)\,dx + \chi_{V_{admissible}}(T), \end{aligned} \tag{2}$$

where χ is the indicator function defined by

$$\chi_{V_{ad}}(T) = \begin{cases} 0 & \text{if } T\in V_{admissible} \\ \infty & \text{if } T\notin V_{admissible} \end{cases}.$$

We consider now the problem (IP):

$$\begin{aligned} \min \int_\Omega &(T-T_d)^2 + \kappa u^2 \\ &- \mu\ln(T-T_{therapeutic}) + \ln(T_{healthy}-T)\,dx + \chi_{V_{ad}}(y) \end{aligned}$$

such that (T,u) fulfill the PDE (1).
Barrier (or Interior-Point) methods are extensively investigated in some recent papers as e.g. [2], [3], such that we summarize here the main results without proof.

Theorem (Existence) The Problem (IP) has for every $\mu > 0$ a unique solution (T_μ, u_μ). The state T_μ touches the bounds only on subsets of Ω with measure zero.

Theorem (Convergence) Let $(T,u)^*$ be the unique minimizer of Problem (HYPER). Then for for every $\mu > 0$ the error estimate

$$\|(T_\mu, u_\mu) - (T,u)^*\| \leq c\sqrt{\mu}$$

holds.

Theorem (Optimality system) Let (T_μ, u_μ) be the unique minimizer of Problem (IP). Assume that T_μ touches the bounds only on subsets of Ω with measure zero. Then there is an adjoint state p such that the pair (T_μ, u_μ) together with p fulfills

- the adjoint equation

$$\begin{aligned} -\nabla\cdot(A\nabla p) + a_0 p = &\int_\Omega \left(T_\mu - T_d\right) v\,dx \\ &- \int_\Omega \frac{\mu}{T_\mu - T_{therapeutic}} v\,dx + \int_\Omega \frac{\mu}{T_{healthy}-T_\mu} v\,dx \quad \text{in } \Omega \\ \vec{n}\nabla Ap + \alpha_0 p = 0 \quad &\text{on } \Gamma, \end{aligned}$$

- the gradient equation

$$\int_\Omega (\kappa u_\mu + p) v\,dx = 0 \;\forall\, v \in L^2(\Omega),$$

and

- the state equation (1)

After transforming the optimality system, we can use a nonlinear complementarity function, e.g. the Fischer-Burmeister function

$$\begin{aligned} \Phi_{FB}(T;\mu) := \\ (T-T_c) + \eta_c - \sqrt{(T-T_c)^2 + \eta_c^2 + 2\mu}, \end{aligned}$$

to implement the complementarity conditions. By $H(T,p,\eta_a,\eta_b;\mu)$ we sample the optimality system in one function.

Path-following algorithm

An algorithm in function spaces for our Barrier method is given by:

Algorithm 1 Barrier Method

Choose $0<\sigma<1$, $0<eps$,
a initial solution $(T,p,\eta_a,\eta_b)^0$ such that
$T_{therapeutic} < T^0 \leq T_{healthy}$. Choose $\mu_0 > 0$. Set $k=0$.
while $\mu_k > eps$
{
$\mu_{k+1} = \sigma\mu_k$
$d^{k+1} = -\partial H((T,p,\eta_a\eta_b)^k;\mu_{k+1})^{-1} H(T,p,\eta_a,\eta_b)^k;\mu_{k+1})$
$(T,p,\eta_a,\eta_b)^{k+1} = (T,p,\eta_a,\eta_b)^k + d^{k+1}$
$k = k+1$
}

Within the while loop we take one Newton step from $(T,p,\eta_a,\eta_b)^k$ in direction $\partial H(T,p,\eta_a,\eta_b)^k$. Having defined the PDEs, implemention of the path-following in COMSOL is quite simple (cf. also [1]):

```
mu=1e-1;
while mu>1e-8,
   mu = mu*0.85;
   fem.const{4} =  num2str(mu);
   fem.xmesh = meshextend(fem);
   fem  = femnlin(fem,...
          'init',fem.sol,...
          'out','fem',...
          'Damping','off',...
          'Maxiter',1);
end
```

Optimal control of the hyperthermia problem

We simplify our patient in the following way: We consider only the part of the body (here the leg) where the tumor is situated. The cut offs of the rest of the body are modeled by do-nothing boundary conditions. We identify the tumor as an ellipsoid inside muscle tissue. We assume the following diffusion and perfusion coefficients:

tissue	a_{ii}	a_0
muscle	0.5	3.8
fat	0.2	1.6
bone	0.3	0.05
tumor	0.2	0.5

Table 1: Thermal conductivity and perfusion coefficients for different kinds of tissue.

The desired temperature and the constraints are defined by

$$T_d = \begin{cases} 45 & x\in\Omega_{tumor} \\ \text{any} & x\in\Omega\backslash\Omega_{tumor} \end{cases},$$

$$T_{therapeutical} = \begin{cases} 45 & x\in\Omega_{tumor} \\ 36 & x\in\Omega\backslash\Omega_{tumor} \end{cases}$$

and

$$T_{healthy} = \begin{cases} 48 & x\in\Omega_{tumor} \\ 41 & x\in\Omega\backslash\Omega_{tumor} \end{cases}.$$

The lower bound T_a guaranties the effect of the hyperthermia, and T_b is a safety bound to protect the patient. Note, that T_d is defined only in Ω_{tumor}. Further, we set the outside temperature $T_b = 36$ and $\alpha_0 = 1.2$.
By using our algorithm we obtain the optimal solution provided in Figure 2.

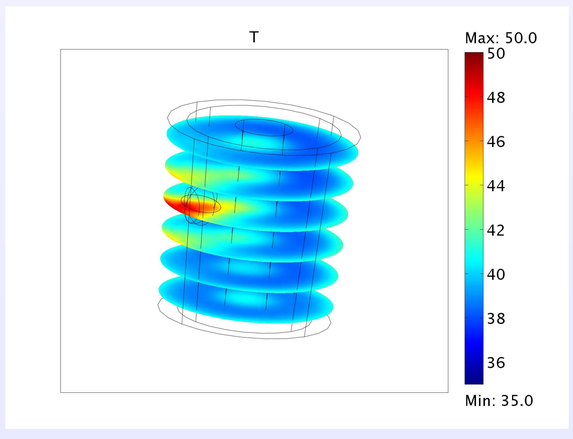

Figure 2: Optimal temperature $T^{\mu_{eps}}$.

The dark blue colored region is muscle tissue with strong blood perfusion. The relatively hot region in the center is caused by the good heat conduction by a coincidental lack of perfusion inside the bone. Figure 3 presents the the optimal heat distribution. Blue colors mark regions where the patient should be cooled.

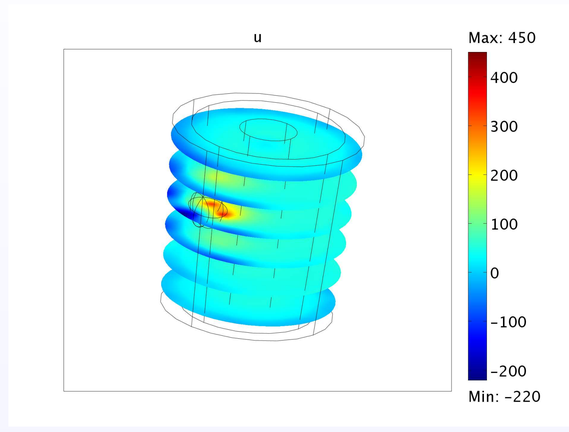

Figure 3: Optimal control $u^{\mu_{eps}}$.

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[3] Anton Schiela. An extended mathematical framework for barrier methods in function space. ZIB-Report 08-07, Konrad-Zuse-Zentrum für Informationstechnik Berlin, 2008.

Contact: Ira Neitzel[1,*], Uwe Prüfert[1,**], Thomas Slawig[2,*].

Institute: [1]Technische Universität Berlin and *SPP 1253, **MATHEON;
[2]Excellence Cluster The Future Ocean, Algorithmic Optimal Control – Oceanic CO_2-Uptake.

Email: neitzel@math.tu-berlin.de,
pruefert@math.tu-berlin.de
ts@informatik.uni-kiel.de