Optimal boundary control of a system of reaction diffusion equations

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Outline

Model problem

Optimality conditions

Numerical examples

$$\min J(u,v,c,d) := \frac{1}{2}\iint\limits_Q (u(x,t)-kv(x,t))^2 \, dxdt + \frac{\lambda_1}{2}\int_0^T c^2(t)\, dt + \frac{\lambda_2}{2}\int_0^T d^2(t)\, dt$$

subject to the system of semilinear parabolic PDE's

$$\begin{aligned}
u_t - D_1 u_{xx} + k_1 u &= -\gamma_1 uv && \text{in } Q := [0,l]\times(0,T),\\
v_t - D_2 v_{xx} + k_2 v &= -\gamma_2 uv && \text{in } Q,\\
u(0,t) - D_1 u_x(0,t) &= c(t) && \text{in } (0,T),\\
D_1 u_x(l,t) &= 0 && \text{in } (0,T),\\
v(0,t) - D_2 v_x(0,t) &= d(t) && \text{in } (0,T),\\
D_2 v_x(l,t) &= 0 && \text{in } (0,T),\\
u(x,0) &= u_0(x) && \text{in } \Omega,\\
v(x,0) &= v_0(x) && \text{in } \Omega
\end{aligned}$$

and the box constraints

$$c \in C_{ad} = \{c \in L^2(0,T) | c_a(t) \le c(t) \le c_b(t) \text{ a.e. in } [0,T]\} \subset L^\infty(0,T),$$

$$d \in D_{ad} = \{d \in L^2(0,T) | d_a(t) \le d(t) \le d_b(t) \text{ a.e. in } [0,T]\} \subset L^\infty(0,T).$$

R. Griesse, *Parametric Sensitivity Analysis for Control-Constraint Optimal Control Problems Governed by Systems of Parabolic Partial Differential Equations*, PhD thesis, University of Bayreuth (2003)

R. Griesse and S. Volkwein, *A primal-dual active set strategy for optimal boundary control of a nonlinear reaction-diffusion system*, SIAM J. CONTROL OPTIM. (2005), Vol. 44, No. 2, pp. 467-494

$\hookrightarrow$ We additionally introduced a nonlinear boundary term.

Domain:

- $\Omega \subset \mathbb{R}^N$, $N \geq 1$,
- Lipschitz-continuous boundary $\Gamma = \partial\Omega$,
- space-time cylinder $Q := \Omega \times (0, T)$,
- $\Sigma := \Gamma \times (0, T)$.

$$
\begin{aligned}
(P) \qquad \min J(u,v,c) \quad = \quad & \frac{\alpha_u}{2}\|u-u_Q\|^2_{L^2(Q)} + \frac{\alpha_v}{2}\|v-v_Q\|^2_{L^2(Q)} + \\
& \frac{\alpha_{TU}}{2}\|u(T)-u_\Omega\|^2_{L^2(\Omega)} + \frac{\alpha_{TV}}{2}\|v(T)-v_\Omega\|^2_{L^2(\Omega)} + \\
& \frac{\alpha_c}{2}\|c\|^2_{L^2(\Sigma)}
\end{aligned}
$$

subject to

$$
(E)\left\{
\begin{array}{rcll}
u_t - D_1\Delta u + k_1 u & = & -\gamma_1 uv & \text{in } Q, \\
v_t - D_2\Delta v + k_2 v & = & -\gamma_2 uv & \text{in } Q, \\
D_1\partial_\nu u + b(x,t,u) & = & c(x,t) & \text{in } \Sigma, \\
D_2\partial_\nu v + \varepsilon v & = & 0 & \text{in } \Sigma, \\
u(x,0) & = & u_0(x) & \text{in } \Omega, \\
v(x,0) & = & v_0(x) & \text{in } \Omega
\end{array}
\right.
$$

and the box constraint

$$
c \in C_{ad} = \{c \in L^\infty(\Sigma) : c_a \le c \le c_b \ a.e.\ in\ \Sigma\}.
$$

Definition

Two pairs of functions $(\tilde{u}, \tilde{v})$ and $(\hat{u}, \hat{v})$ in $C(\overline{Q}) \cap C^{1,2}(Q)$ are called ordered upper and lower solutions of (E), if $(\tilde{u}, \tilde{v})(x,t) \geq (\hat{u}, \hat{v})(x,t)$ in $\overline{Q}$ and the following inequalities are satisfied:

$$
\begin{array}{rcccll}
\tilde{u}(x,0) & \geq & u_0(x) & \geq & \hat{u}(x,0) & \text{in } \Omega \\
\tilde{v}(x,0) & \geq & v_0(x) & \geq & \hat{v}(x,0) & \text{in } \Omega \\
D_1 \partial_\nu \tilde{u} - c + b(x,t,\tilde{u}) & \geq & 0 & \geq & D_1 \partial_\nu \hat{u} - c + b(x,t,\hat{u}) & \text{in } \Sigma \\
D_2 \partial_\nu \tilde{v} + \varepsilon \tilde{v} & \geq & 0 & \geq & D_2 \partial_\nu \hat{v} + \varepsilon \hat{v} & \text{in } \Sigma \\
\tilde{u}_t - D_1 \Delta \tilde{u} + k_1 \tilde{u} + \gamma_1 \tilde{u} \hat{v} & \geq & 0 & \geq & \hat{u}_t - D_1 \Delta \hat{u} + k_1 \hat{u} + \gamma_1 \hat{u} \tilde{v} & \text{in } Q \\
\tilde{v}_t - D_2 \Delta \tilde{v} + k_2 \tilde{v} + \gamma_2 \hat{u} \tilde{v} & \geq & 0 & \geq & \hat{v}_t - D_2 \Delta \hat{v} + k_2 \hat{v} + \gamma_2 \tilde{v} \hat{v} & \text{in } Q.
\end{array}
$$

Theorem (Pao)

Let $(\tilde{u}, \tilde{v})$ und $(\hat{u}, \hat{v})$ be ordered upper and lower solutions of (E), $(-\gamma_1 uv, -\gamma_2 uv)$ be quasimonotone nonincreasing in $[(\tilde{u}, \tilde{v}), (\hat{u}, \hat{v})] := \{(u, v) \in C(\overline{Q}) \times C(\overline{Q}) : \tilde{u} \leq u \leq \hat{u} \text{ and } \tilde{v} \leq v \leq \hat{v}\}$ and locally Lipschitz. Then the system (E) has a unique solution (u_1, u_2) in $[(\tilde{u}, \tilde{v}), (\hat{u}, \hat{v})]$, satisfying the relation

$$(\hat{u}, \hat{v}) \leq (u, v) \leq (\tilde{u}, \tilde{v}) \qquad \forall k = 1, 2, \ldots on\ Q.$$

Assumption (**A1**): The nonlinear function $b : \Sigma \times \mathbb{R} \to \mathbb{R}$ is continuous, locally Lipschitz in u of order 2, monotone nondecreasing with respect to u for almost all $(x, t) \in \Sigma$ and fullifies $b(x, t, 0) \leq c_a(x, t)$ for all $(x, t) \in \Sigma$ and $|b(x, t, 0)| + |\nabla b(x, t, 0)| + |b''(x, t, 0)| \leq K$ for almost all $(x, t) \in \Sigma$ with a constant K and $\lim_{u \to \pm\infty} b(x, t, u) = \pm\infty$.

Theorem

For every function $c \in C(\Sigma)$ with $c(x,t) \geq c_a(x,t)$ for all $(x,t) \in \Sigma$, where $c_a \in L^\infty(\Sigma)$ is the lower control constraint, and $u_0, v_0 \in C(\overline{\Omega})$, there exists an unique solution $(u,v) \in \left(C(\overline{Q}) \cap C^{1,2}(Q)\right)^2$ for (E).

PROOF: We first have to find pairs of ordered upper and lower solution:

1. lower solution: $(\hat{u}, \hat{v}) = (0,0)$,
2. upper solution: $(\tilde{u}, \tilde{v}) = (\delta, \delta)$,

where $\delta := \max(\delta_v, \delta_u)$ and δ_u, δ_v are positive constants satisfying

$$\delta_u \geq u_0(x), \;\; \delta_v \geq v_0(x) \quad \forall x \in \Omega, \tag{1}$$

and

$$b(x,t,\delta_u) \geq c(x,t) \quad \forall (x,t) \in \Sigma. \tag{2}$$

We derive the existence of these constants, because of Assumption **A1**. The conditions (1) and (2) can be satisfied since $u_0, v_0 \in C(\overline{\Omega})$ and the assumptions **A1** on b hold.

Theorem

For every given $c \in C_{ad}$, there exists a unique weak solution $(u, v) \in Y^2 := \left(W(0,T) \cap C(\overline{Q})\right)^2$ of (E).

Sketch of proof [Existence]:

- $c \in C_{ad} \subset L^\infty(\Sigma),\ c_a \le c_n \in C(\Sigma),\ c_n \to c \in L^s(\Sigma),\ s > N+1,$
- For every c_n, we choose the same upper and lower solutions, since all c_n are uniformly bounded
  $(\hat{u}, \hat{v}) \le (u_n, v_n) \le (\tilde{u}, \tilde{v}) \quad \forall n = 1, 2, \dots$ in Q,
- so an $M > 0$ exists with $\|u_n\|_{C(\overline{Q})} + \|v_n\|_{C(\overline{Q})} \le M$,
- define $h_n := c_n - b(\cdot, u_n)$ and $g_n := g(u_n, v_n) = -\gamma_1 u_n v_n$,
- h_n, g_n are uniformly bounded in $L^\infty(Q)$, hence in $L^s(Q), L^r(Q)$, $r > N/2 + 1$ (weakly convergence),

$$\begin{aligned}(u_n)_t - D_1 \Delta u_n + k_1 u_n &= g_n \\ D_1 \partial_\nu u_n &= h_n \\ u_n(x,0) &= u_0(x).\end{aligned} \quad (3)$$

- possess for all $(g_n, h_n) \in L^r(Q) \times L^s(\Sigma)$ a unique solution u_n in Y,
- control-to-state mapping is continuous (i.e. Casas,Raymond,Zidani),
- also weak continuous (linearity) $\Rightarrow u_n \rightharpoonup u$ in Y,
- at the end we show that $u \in Y$ and $v \in Y$, obtained analogously, satisfy the state equation

Theorem

Problem (P) admits at least one optimal control $\bar{c}$.

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To formulate necessary optimality conditions, let $\overline{c}$ be an optimal control of (P) with optimal states $(\overline{u}, \overline{v})$. Then there exist $(p, q) \in W(0,T) \times W(0,T)$ which are weak solutions to the **adjoint equations:**

$$(A)\left\{\begin{array}{rcll} -p_t - D_1\Delta p + k_1 p + \gamma_1 \overline{v} p + \gamma_2 \overline{v} q &=& \alpha_u(\overline{u} - u_Q) & \text{in } Q, \\ -q_t - D_2\Delta q + k_2 q + \gamma_1 \overline{u} p + \gamma_2 \overline{u} q &=& \alpha_v(\overline{v} - v_Q) & \text{in } Q, \\ D_1 \partial_\nu p + b_u(x,t,\overline{u}) p &=& 0 & \text{in } \Sigma, \\ D_2 \partial_\nu q + \varepsilon q &=& 0 & \text{in } \Sigma, \\ p(x,T) = \alpha_{TU}(\overline{u}(x,T) - u_\Omega(x)) & & & \text{in } \Omega, \\ q(x,T) = \alpha_{TV}(\overline{v}(x,T) - v_\Omega(x)) & & & \text{in } \Omega. \end{array}\right.$$

Every locally optimal solution $\overline{c}$ of (P) satisfies, together with the adjoint states (p, q) of (A), the variational inequality

$$\int_{\Sigma} (p + \alpha_c \overline{c})(c - \overline{c}) \; dt \;\geq\; 0 \qquad \forall c \in C_{ad}.$$

For $\alpha_c > 0$, this leads to the projection formula

$$\overline{c}(x,t) = P_{[c_a(x,t), c_b(x,t)]}\{-\frac{1}{\alpha_c} p(x,t)\}$$

for almost all $(x, t) \in \Sigma$.
This leads to

$$\overline{c} = \begin{cases} c_a, \text{ if } p + \alpha_c \overline{c}(t) > 0 \\ c_b, \text{ if } p + \alpha_c \overline{c}(t) < 0. \end{cases} \tag{4}$$

By the first-order conditions, the control function $\overline{c}$ is defined in the set $\{(x,t) \in \Sigma : |p + \alpha_c \overline{c}| > 0\}$. Therefor, second-order sufficient conditions should be required on the remaining sets. For given $\tau > 0$, we define

$$A_\tau(\overline{c}) := \{(x,t) \in \Sigma : |p + \alpha_c \overline{c}| > \tau\}$$

as the *set of strongly active restrictions* for $\overline{c}$. The *τ-citical cone* $C_\tau(\overline{c})$ is made up of all $c \in L^\infty(\Sigma)$ with

$$c(x,t) \begin{cases} = 0 & \text{for } (x,t) \in A_\tau(\overline{c}) \\ \geq 0 & \text{for } \overline{c}(x,t) = c_a \text{ and } (x,t) \notin A_\tau(\overline{c}) \\ \leq 0 & \text{for } \overline{c}(x,t) = c_b \text{ and } (x,t) \notin A_\tau(\overline{c}). \end{cases}$$

Remark

This is the cone appearing in anatural way for second-order necessary conditions. In the case of sufficient conditions, where the L^2-norm occurs, one might consider also the same cone in L^2. This however, will not give new conditions by density of L^∞ in L^2.

Theorem (SSC)

Suppose that the control function $\overline{c}$ satisfies the first-order necessary optimality conditions. If there exist positive constants δ and τ such that

$$\mathcal{L}''(\overline{u}, \overline{v}, \overline{c}, p, q)(u, v, c)^2 \geq \delta \|c\|^2_{L^2(0,T)}$$

holds for all $c \in C_\tau(\overline{c})$ and all $(u, v) \in Y \times Y$ satisfying the linearized state equation, then we find positive constants ε and σ such that

$$J(u, v, c) \geq J(\overline{u}, \overline{v}, \overline{c}) + \sigma \|c - \overline{c}\|^2_{L^2(Q)}$$

holds for all $c \in C_{ad}$ with $\|c - \overline{c}\|_{L^\infty(Q)} \leq \varepsilon$. Therefore, the control function $\overline{c}$ is locally optimal.

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Inserting the projection formula in the system (E), we obtain a nonlinear and non-smooth coupled system of parabolic equations:

$$\begin{aligned} u_t - D_1 \Delta u + k_1 u &= -\gamma_1 uv \\ D_1 \partial_\nu u + b(x,t,u) &= P_{[c_a(x,t),c_b(x,t)]}\{-\frac{1}{\alpha_c} p(x,t)\} \\ u(x,0) &= u_0(x) \\ v_t - D_2 \Delta v + k_2 v &= -\gamma_2 uv \\ D_2 \partial_\nu v + \varepsilon v &= 0 \\ v(x,0) &= v_0(x) \end{aligned}$$

+ the system of adjoint equations (A).

Example 1:

$\Omega = [0,1] \times [0,1], \;\; T = 5,$
$D_1 = D_2 = k_1 = k_2 = 1,$
$\gamma_1 = \gamma_2 = 0.3,$
$\alpha_{TU} = \alpha_{TV} = 10, \; \alpha_u = \alpha_v = 0, \; \alpha_c = 0.01,$
$\varepsilon = 0.1, \; u_0(x) = 0, \; v_0(x) = 100,$
$u_\Omega = \sin(2\pi x) + 1, \; v_\Omega = 1.$
$c_a \equiv 0, \; c_b \equiv 20,$
$b = u^4.$

We solved the whole system with COMSOL MULTIPHISICS (a registered trademark of Comsol Ab) in about 15 seconds (about 10000 degrees of freedom).

We consider the time as the third space dimension.
(Idea by I.Neitzel, U.Prüfert and T.Slawig)

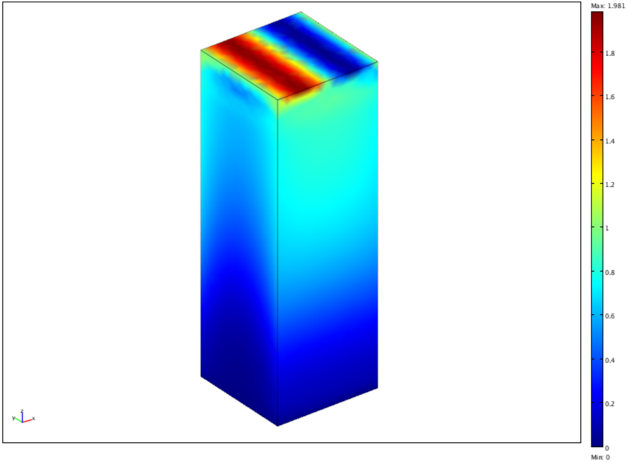


Figure: State u for Example 1

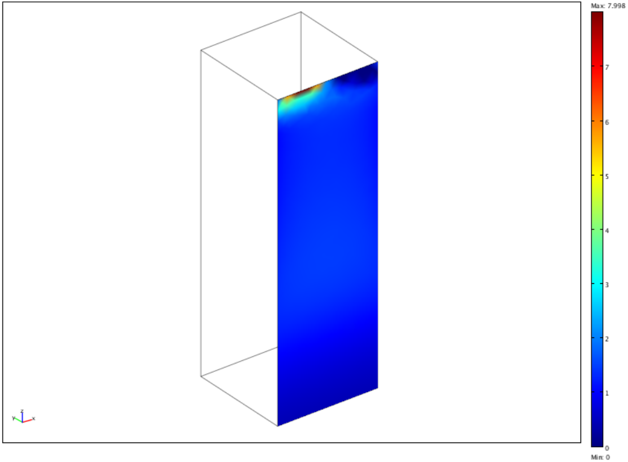


Figure: Optimal control $\overline{c}$ for Example 1

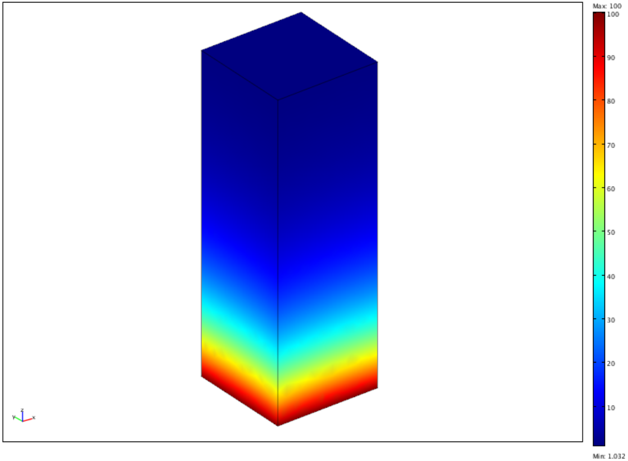
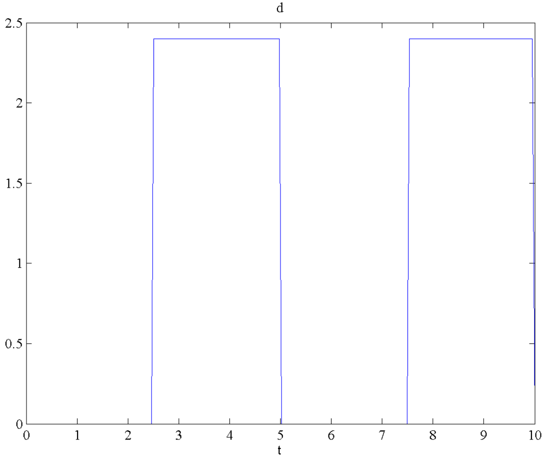


Figure: State v for Example 1

Example 2:



Setting $\Omega = [0,1]$, $T = 10$, $k = D_1 = D_2 = 1$, $\gamma_1 = \gamma_2 = 0.5$
$k_1 = k_2 = 0.3$, $\lambda_1 = \lambda_2 = 0.001$, $d_0 = 7$, $u_0 = v_0 \equiv 0$ and for the control constraints c

$$c_a(t) = \begin{cases} 0 \text{ on } [T/4, T/2[\cup [3T/4, T[\\ 1 \text{ on } [0, T/4[\cup [T/2, 3T/4[\end{cases}$$

and

$$c_b(t) = \begin{cases} 0 \text{ on } [T/4, T/2[\cup [3T/4, T[\\ 10 \text{ on } [0, T/4[\cup [T/2, 3T/4[. \end{cases}$$

We solved the whole system with COMSOL MULTIPHISICS (a registered trademark of Comsol Ab) in about 2 seconds (about 3500 degrees of freedom). And with a gradient-projection-method with finite-differences and implizit euler in 12 seconds (about 20000 degrees of freedom).

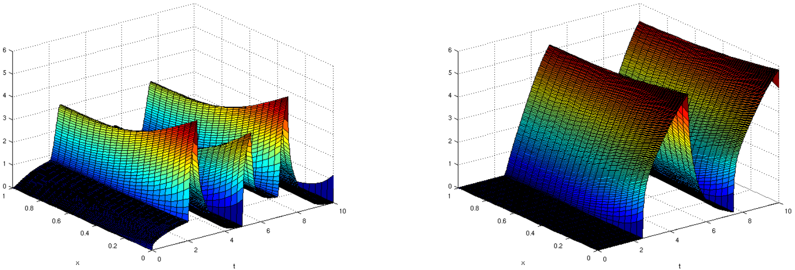


Figure: State u and v for Example 2

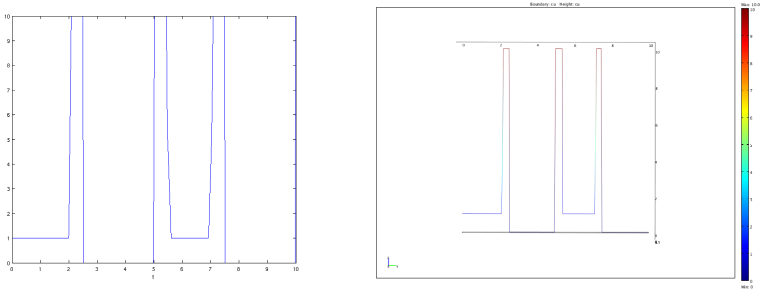


Figure: Optimal control $\overline{c}$: GP and COMSOL for Example 2