Optimal control of Allen–Cahn equations with singular potentials and dynamic boundary conditions

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(joint work with P. Colli)
The optimal control problem

Consider the IVP with dynamic boundary condition

\[ y_t - \Delta y + f'(y) = u \quad \text{a.e. in } Q, \]  
\[ \partial_t y_{\Gamma} - \Delta_{\Gamma} y_{\Gamma} + \partial_n y + g'(y_{\Gamma}) = u_{\Gamma}, \quad y_{\Gamma} = y_{\Gamma}, \quad \text{a.e. on } \Sigma, \]  
\[ y(0) = y_0 \quad \text{a.e. in } \Omega, \quad y_{\Gamma}(0) = y_{0\Gamma} \quad \text{a.e. on } \Gamma. \]  

Here, we have

- \( \Delta_{\Gamma} \): Laplace–Beltrami operator, \( n \): outward unit normal derivative;
- \( f, g \): given nonlinearities;
- \( u, u_{\Gamma} \): control functions;
- \( y_0 \in H^1(\Omega) \): initial datum s.t. \( y_0|_{\Gamma} = y_{0\Gamma} \).
The optimal control problem

We introduce the Banach spaces

\[ H := L^2(\Omega), \quad V := H^1(\Omega), \quad H_\Gamma := L^2(\Gamma), \quad V_\Gamma := H^1(\Gamma), \]
\[ \mathcal{H} := L^2(Q) \times L^2(\Sigma), \quad \mathcal{X} := L^\infty(Q) \times L^\infty(\Sigma), \]
\[ \mathcal{Y} := \left\{ (y, y_\Gamma) : y \in H^1(0, T; H) \cap C^0([0, T]; V) \cap L^2(0, T; H^2(\Omega)), \right. \]
\[ \left. y_\Gamma \in H^1(0, T; H_\Gamma) \cap C^0([0, T]; V_\Gamma) \cap L^2(0, T; H^2(\Gamma)), \quad y_\Gamma = y|_\Gamma \right\}, \]

endowed with their respective natural norms. We also assume:

**(A1)** There are given functions

\[ z_Q \in L^2(Q), \quad z_\Sigma \in L^2(\Sigma), \quad z_T \in V, \quad z_\Gamma, z_T \in V_\Gamma, \]
\[ \tilde{u}_1, \tilde{u}_2 \in L^\infty(Q) \text{ with } \tilde{u}_1 \leq \tilde{u}_2 \text{ a.e. in } Q, \]
\[ \tilde{u}_{1\Gamma}, \tilde{u}_{2\Gamma} \in L^\infty(\Sigma) \text{ with } \tilde{u}_{1\Gamma} \leq \tilde{u}_{2\Gamma} \text{ a.e. on } \Sigma. \]
The optimal control problem

(1) Minimize the (tracking-type) cost functional

\[ J((y, y_\Gamma), (u, u_\Gamma)) := \frac{\beta_1}{2} \int_0^T \int_\Omega |y - z_Q|^2 \, dx \, dt + \frac{\beta_2}{2} \int_0^T \int_\Gamma |y_\Gamma - z_\Sigma|^2 \, d\Gamma \, dt \]

\[ + \frac{\beta_3}{2} \int_\Omega |y(\cdot, T) - z_T|^2 \, dx + \frac{\beta_4}{2} \int_\Gamma |y_\Gamma(\cdot, T) - z_{\Gamma, T}|^2 \, d\Gamma \]

\[ + \frac{\beta_5}{2} \int_0^T \int_\Omega |u|^2 \, dx \, dt + \frac{\beta_6}{2} \int_0^T \int_\Gamma |u_\Gamma|^2 \, d\Gamma \, dt \] (4)

subject to the state system (1)–(3) and to the control constraint

\[ (u, u_\Gamma) \in \mathcal{U}_{ad} := \{ (w, w_\Gamma) \in \mathcal{H} : \tilde{u}_1 \leq w \leq \tilde{u}_2 \text{ a.e. in } Q, \]

\[ \tilde{u}_{1\Gamma} \leq w_\Gamma \leq \tilde{u}_{2\Gamma} \text{ a.e. on } \Sigma \} \] (5)
General assumptions

\((A2)\) \[ f = f_1 + f_2, \quad g = g_1 + g_2, \quad \text{where} \quad f_2, g_2 \in C^3[0, 1], \quad \text{and where} \]
\[ f_1, g_1 \in C^3(0, 1) \quad \text{are convex and satisfy:} \]
\[ \lim_{r \searrow 0} f_1'(r) = \lim_{r \searrow 0} g_1'(r) = -\infty, \quad \lim_{r \nearrow 1} f_1'(r) = \lim_{r \nearrow 1} g_1'(r) = +\infty \quad (6) \]
\[ \exists M_1 \geq 0, M_2 > 0 : \quad |f_1'(r)| \leq M_1 + M_2 |g_1'(r)| \quad \forall r \in (0, 1). \quad (7) \]
General assumptions

(A2) \( f = f_1 + f_2, \quad g = g_1 + g_2, \) where \( f_2, g_2 \in C^3[0,1] \), and where \( f_1, g_1 \in C^3(0,1) \) are convex and satisfy:

\[
\lim_{r \downarrow 0} f_1'(r) = \lim_{r \downarrow 0} g_1'(r) = -\infty, \quad \lim_{r \uparrow 1} f_1'(r) = \lim_{r \uparrow 1} g_1'(r) = +\infty \tag{6}
\]

\[\exists \ M_1 \geq 0, \ M_2 > 0 : \quad |f_1'(r)| \leq M_1 + M_2 |g_1'(r)| \quad \forall r \in (0,1). \tag{7}\]

(A3) \( y_0 \in V, \quad y_{0|\Gamma} = y_{0|\Gamma}, \quad f_1(y_0) \in L^1(\Omega), \quad g_1(y_{0|\Gamma}) \in L^1(\Gamma), \) and

\[0 < y_0 < 1 \quad \text{a.e. in } \Omega, \quad 0 < y_{0|\Gamma} < 1 \quad \text{a.e. on } \Gamma. \tag{8}\]
General assumptions

(A2) \( f = f_1 + f_2, \ g = g_1 + g_2, \) where \( f_2, g_2 \in C^3[0,1] \), and where \( f_1, g_1 \in C^3(0,1) \) are convex and satisfy:

\[
\lim_{r \rightarrow 0} f_1'(r) = \lim_{r \rightarrow 0} g_1'(r) = -\infty, \quad \lim_{r \rightarrow 1} f_1'(r) = \lim_{r \rightarrow 1} g_1'(r) = +\infty \tag{6}
\]

\[
\exists M_1 \geq 0, M_2 > 0 : \quad |f_1'(r)| \leq M_1 + M_2 |g_1'(r)| \quad \forall r \in (0,1). \tag{7}
\]

(A3) \( y_0 \in V, \ y_0|_{\Gamma} = y_0|_{\Gamma}, \ f_1(y_0) \in L^1(\Omega), \ g_1(y_0|_{\Gamma}) \in L^1(\Gamma), \) and

\[
0 < y_0 < 1 \text{ a.e. in } \Omega, \quad 0 < y_0|_{\Gamma} < 1 \text{ a.e. on } \Gamma. \tag{8}
\]

(A4) \( \mathcal{U} \subset \mathcal{X} \) is open such that \( \mathcal{U}_{ad} \in \mathcal{U} \), and there is some \( R > 0 \) with

\[
\|u\|_{L^\infty(Q)} + \|u_{\Gamma}\|_{L^\infty(\Sigma)} \leq R \quad \forall (u,u_{\Gamma}) \in \mathcal{U}. \tag{9}
\]
Remarks:

1. (A2) implies that the singularity on the boundary grows at least with the same order as the one in the bulk.
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2. Typical nonlinearities satisfying (5) and (6) are

\[
f_1(r) = c_1(r \log(r) + (1 - r) \log(1 - r)),
\]

\[
g_1(r) = c_2(r \log(r) + (1 - r) \log(1 - r)),
\]

where \( c_1 > 0, c_2 > 0 \).
General assumptions

Remarks:

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2. Typical nonlinearities satisfying (5) and (6) are

\[ f_1(r) = c_1(r \log(r) + (1 - r) \log(1 - r)), \]
\[ g_1(r) = c_2(r \log(r) + (1 - r) \log(1 - r)), \]

where \( c_1 > 0, c_2 > 0 \).

3. We assume here a differentiable situation. The results are submitted to SIAM J. Control Optimization. A non-differentiable case is studied in Colli–Farshbaf-Shaker–Sprekels (in preparation): there, we assume that \( f_1 = g_1 = I_{[0,1]} \), so that we have to replace \( f_1' \), \( g_1' \) in (1) and (2) by the subdifferential \( \partial I_{[0,1]} \).
The state system

The following result is a special case of results proved in Calatroni–Colli (Nonlinear Anal. 2013):

**Theorem 1:** Suppose that (A2), (A3) are satisfied. Then we have:

(i) The state system (1)–(3) has for any \((u, u_\Gamma) \in H\) a unique solution \((y, y_\Gamma) \in \mathcal{Y}\) such that

\[
0 < y < 1 \quad \text{a.e. in } Q, \quad 0 < y_\Gamma < 1 \quad \text{a.e. on } \Sigma.
\] (10)

(ii) If also (A4) holds, \(\exists K^*_1 > 0\): for any \((u, u_\Gamma) \in \mathcal{U}\) the associated solution \((y, y_\Gamma) \in \mathcal{Y}\) satisfies

\[
\|(y, y_\Gamma)\|_{\mathcal{Y}} \leq K^*_1, \quad \|f'(y)\|_{L^2(Q)} + \|g'(y_\Gamma)\|_{L^2(\Sigma)} \leq K^*_1.
\] (11)

Moreover, \(\exists K^*_2 > 0\): whenever \((u_1, u_{1\Gamma}), (u_2, u_{2\Gamma}) \in \mathcal{U}\) are given, then we have

\[
\|y_1 - y_2\|_{C^0([0,T];H)} + \|\nabla (y_1 - y_2)\|_{L^2(Q)} + \|y_{1\Gamma} - y_{2\Gamma}\|_{C^0([0,T];H_\Gamma)}
\]
\[
+ \|\nabla_\Gamma (y_{1\Gamma} - y_{2\Gamma})\|_{L^2(\Sigma)}
\]
\[
\leq K^*_2 \left(\|u_1 - u_2\|_{L^2(Q)} + \|u_{1\Gamma} - u_{2\Gamma}\|_{L^2(\Sigma)}\right).
\] (12)
Remark:

4. Owing to Theorem 1, the control-to-state mapping

\[ S : (u, u_\Gamma) \mapsto S(u, u_\Gamma) := (y, y_\Gamma) \]

is defined as a mapping from \( \mathcal{H} \) into \( \mathcal{Y} \). Moreover, \( S \) is Lipschitz continuous when viewed as a mapping from the subset \( U \) of \( \mathcal{H} \) into the space \( (C^0([0, T]; H) \cap L^2(0, T; V)) \times (C^0([0, T]; H_\Gamma) \cap L^2(0, T; V_\Gamma)) \).

We now come to a linearized version of Theorem 1, which will play a central role in the derivation of first-order necessary and second-order sufficient conditions for (CP).
Theorem 2: Let \((u, u_\Gamma) \in \mathcal{H}, \ c_1 \in L^\infty(Q), \ c_2 \in L^\infty(\Sigma)\), as well as
\[(w_0, w_0\Gamma) \in V \times V_\Gamma \text{ with } w_0|\Gamma = w_0\Gamma \text{ be given. Then we have:}\]

(i) The linear IBVP

\[
\begin{align*}
    w_t - \Delta w + c_1(x, t) w &= u \quad \text{a.e. in } Q, \\
    \partial_t w_\Gamma - \Delta_\Gamma w_\Gamma + \partial_n w + c_2(x, t) w_\Gamma &= u_\Gamma, \quad w|\Gamma = w_\Gamma, \quad \text{a.e. on } \Sigma, \\
    w(\cdot, 0) &= w_0 \quad \text{a.e. in } \Omega, \quad w_\Gamma(\cdot, 0) = w_0\Gamma \quad \text{a.e. on } \Gamma,
\end{align*}
\]

has a unique solution \((w, w_\Gamma) \in \mathcal{Y}\).

(ii) There is some \(\hat{C} > 0\) such that: whenever \(w_0 = 0\) and \(w_0\Gamma = 0\) then

\[
\|(w, w_\Gamma)\|_\mathcal{Y} \leq \hat{C} \|(u, u_\Gamma)\|_\mathcal{H}.
\]
A linear system

Idea of Proof: (i) is more or less a consequence of Theorem 1. Now let $w_0 = 0$, $w_0^{\Gamma} = 0$. Testing (13) by $w_t$ and applying Young’s and Gronwall’s inequalities, we easily find

$$\|w\|_{H^1(0,T;H)} \cap C^0([0,T];V) + \|w^{\Gamma}\|_{H^1(0,T;H^{\Gamma})} \cap C^0([0,T];V^{\Gamma}) \leq C_1 \|(u,u^{\Gamma})\|_H.$$  

Comparison in (13) yields

$$\|\Delta w\|_{L^2(Q)} \leq C_2 \|(u,u^{\Gamma})\|_H.$$  

Then, applying a standard embedding result,

$$\|w\|_{L^2(0,T;H^{3/2}(\Omega))} \leq C_3 \|(u,u^{\Gamma})\|_H,$$

whence, by the trace theorem,

$$\|\partial_n w\|_{L^2(0,T;H^{\Gamma})} \leq C_4 \|(u,u^{\Gamma})\|_H.$$
A linear system

But then, by comparison in (14),

$$\|\Delta \Gamma w_{\Gamma}\|_{L^2(\Sigma)} \leq C_5 \|(u, u_{\Gamma})\|_H,$$

whence

$$\|w_{\Gamma}\|_{L^2(0,T;H^2(\Gamma))} \leq C_6 \|(u, u_{\Gamma})\|_H.$$

Standard elliptic estimates then yield

$$\|w\|_{L^2(0,T;H^2(\Omega))} \leq C_7 \|(u, u_{\Gamma})\|_H.$$ 

Remark:

5. It cannot be expected that \((w, w_{\Gamma}) \in L^\infty(Q) \times L^\infty(\Sigma),\) in general.
An $L^\infty$ bound for $(y, y_\Gamma)$

(A5) It holds $y_0 \in L^\infty(\Omega)$, $y_{0r} \in L^\infty(\Gamma)$, as well as

$$0 < \text{ess inf } y_0(x), \quad \text{ess sup } y_0(x) < 1, \quad x \in \Omega$$

$$0 < \text{ess inf } y_{0r}(x), \quad \text{ess sup } y_{0r}(x) < 1, \quad x \in \Gamma$$
An $L^\infty$ bound for $(y, y_\Gamma)$

(A5) It holds $y_0 \in L^\infty(\Omega)$, $y_{0\Gamma} \in L^\infty(\Gamma)$, as well as

\[ 0 < \text{ess inf}_{x \in \Omega} y_0(x), \quad \text{ess sup}_{x \in \Omega} y_0(x) < 1, \]

\[ 0 < \text{ess inf}_{x \in \Gamma} y_{0\Gamma}(x), \quad \text{ess sup}_{x \in \Gamma} y_{0\Gamma}(x) < 1. \]

Lemma 3: Let (A2)--(A5) hold. Then $\exists 0 < r_* < r^* < 1$ such that:

whenever $(y, y_\Gamma) = S(u, u_\Gamma)$ for some $(u, u_\Gamma) \in \mathcal{U}$, then it holds

\[ r_* \leq y \leq r^* \text{ a.e. in } Q, \quad r_* \leq y_\Gamma \leq r^* \text{ a.e. on } \Sigma. \] (17)
An $L^\infty$ bound for $(y, y_\Gamma)$

(A5) It holds $y_0 \in L^\infty(\Omega), y_{0\Gamma} \in L^\infty(\Gamma)$, as well as

$$0 < \text{ess inf}_{x \in \Omega} y_0(x), \quad \text{ess sup}_{x \in \Omega} y_0(x) < 1,$$

$$0 < \text{ess inf}_{x \in \Gamma} y_{0\Gamma}(x), \quad \text{ess sup}_{x \in \Gamma} y_{0\Gamma}(x) < 1.$$

Lemma 3: Let (A2)–(A5) hold. Then $\exists 0 < r_* < r^* < 1$ such that:

whenever $(y, y_\Gamma) = S(u, u_\Gamma)$ for some $(u, u_\Gamma) \in \mathcal{U}$, then it holds

$$r_* \leq y \leq r^* \text{ a.e. in } Q, \quad r_* \leq y_\Gamma \leq r^* \text{ a.e. on } \Sigma.$$  (17)

Remark:

6. In view of (A2) and Lemma 3, we may assume that

$$\max_{0 \leq i \leq 3} \left\{ \max \left\{ \| f^{(i)}(y) \|_{L^\infty(Q)}, \| g^{(i)}(y) \|_{L^\infty(\Sigma)} \right\} \right\} \leq K_1^*,$$  (18)

whenever $(y, y_\Gamma) = S(u, u_\Gamma)$ for some $(u, u_\Gamma) \in \mathcal{U}$. 
An $L^\infty$ bound for $(y, y_\Gamma)$

**Proof:** There are constants $0 < r_* \leq r* < 1$ such that

$$r_* \leq \min \left\{ \essinf_{x \in \Omega} y_0(x), \essinf_{x \in \Gamma} y_{0\Gamma}(x) \right\},$$

$$r* \geq \max \left\{ \esssup_{x \in \Omega} y_0(x), \esssup_{x \in \Gamma} y_{0\Gamma}(x) \right\},$$

$$\max \{ f'(r) + R, g'(r) + R \} \leq 0 \ \forall r \in (0, r_*),$$

$$\min \{ f'(r) - R, g'(r) - R \} \geq 0 \ \forall r \in (r*, 1).$$

Now define $w := (y - r*)^+$. Clearly, we have $w \in V$ and $w\rvert_{\Gamma} \in V_{\Gamma}$. We put $w_{\Gamma} := w\rvert_{\Gamma}$ and test (1) by $w$. We readily see that

$$0 = \frac{1}{2} \|w(T)\|_{H}^2 + \int_{0}^{T} \|\nabla w(t)\|_{H}^2 \, dt + \int_{0}^{T} \|\nabla_{\Gamma} w_{\Gamma}(t)\|_{H_{\Gamma}}^2 \, dt + \frac{1}{2} \|w_{\Gamma}(T)\|_{H_{\Gamma}}^2 + \Phi,$$
An $L^\infty$ bound for $(y, y_\Gamma)$

where

$$
\Phi := \int_0^T \int_\Omega (f'(y) - u) \, w \, dx \, dt + \int_0^T \int_\Gamma (g'(y_\Gamma) - u_\Gamma) \, w_\Gamma \, d\Gamma \, dt \geq 0.
$$

In conclusion, $w = (y - r^*)^+ = 0$, i.e., $y \leq r^*$, almost everywhere in $Q$ and on $\Sigma$. The remaining inequalities follow similarly by testing (1) with $w := -(y - r^*)^-$. 

**Remark:**

7. Assume (A2)–(A5) are satisfied. Using arguments similar to those in the proof of (16), we are able to improve the stability estimate (12); $\exists \, K^*_3 > 0$:

whenever $(y_i, y_{i\Gamma}) = S(u_i, u_{i\Gamma})$ for $(u_i, u_{i\Gamma}) \in U$, $i = 1, 2$, then

$$
\|(y_1, y_{1\Gamma}) - (y_2, y_{2\Gamma})\|_Y \leq K^*_3 \|(u_1, u_{1\Gamma}) - (u_2, u_{2\Gamma})\|_H.
$$

This higher Lipschitz continuity is needed to show the Fréchet differentiability of the control-to-state mapping $S$. 

Existence of optimal controls

**Theorem 4:** Suppose that \((A1)-(A4)\) are fulfilled. Then \((CP)\) has a solution.
Existence of optimal controls

**Theorem 4:** Suppose that (A1)–(A4) are fulfilled. Then (CP) has a solution.

**Proof:** Pick a minimizing sentence \( \{(u_n, u_{n\Gamma})\} \subset U_{ad} \), and let

\[
(y_n, y_{n\Gamma}) = S(u_n, u_{n\Gamma}), \ n \in \mathbb{N}.
\]

By the a priori estimates, we may assume that

\[
\begin{align*}
    u_n &\to \bar{u} \text{ weakly-* in } L^\infty(Q),
    u_{n\Gamma} &\to \bar{u}_\Gamma \text{ weakly-* in } L^\infty(\Sigma), \\
    y_n &\to \bar{y} \text{ weakly-* in } H^1(0, T; H) \cap L^\infty(0, T; V) \cap L^2(0, T; H^2(\Omega)) \cap L^\infty(Q), \\
    y_{n\Gamma} &\to \bar{y}_\Gamma \text{ weakly-* in } H^1(0, T; H_\Gamma) \cap L^\infty(0, T; V_\Gamma) \cap L^2(0, T; H^2(\Gamma)) \cap L^\infty(\Sigma).
\end{align*}
\]

In particular, we have (by compact embedding)

\[
\begin{align*}
    y_n &\to \bar{y} \text{ strongly in } C^0([0, T]; H), \\
    y_{n\Gamma} &\to \bar{y}_\Gamma \text{ strongly in } C^0([0, T]; H_\Gamma).
\end{align*}
\]

Passage to the limit \( n \to \infty \) in (1)–(3) easily shows that \( (\bar{y}, \bar{y}_\Gamma) = S(\bar{u}, \bar{u}_\Gamma) \), and the weak sequential lower semicontinuity of \( J \) yields that \( ((\bar{u}, \bar{u}_\Gamma), (\bar{y}, \bar{y}_\Gamma)) \) is an optimal pair.
**Theorem 5:** Suppose that (A2)–(A5) hold. Then we have

(i) Let \((\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}\) be arbitrary. Then \(S : \mathcal{X} \rightarrow \mathcal{Y}\) is Fréchet differentiable at \((\bar{u}, \bar{u}_\Gamma)\), and the Fréchet derivative \(DS(\bar{u}, \bar{u}_\Gamma)\) is given by \(DS(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma) = (\xi, \xi_\Gamma)\), where for any given \((h, h_\Gamma) \in \mathcal{X}\) the pair \((\xi, \xi_\Gamma) \in \mathcal{Y}\) solves the linearized system

\[
\begin{align*}
\xi_t - \Delta \xi + f''(\bar{y}) \xi &= h \quad \text{a.e. in } Q, \\
\partial_t \xi_\Gamma - \Delta_\Gamma \xi_\Gamma + \partial_n \xi + g''(\bar{y}_\Gamma) \xi_\Gamma &= h_\Gamma, \quad \xi_\Gamma = \xi|_\Gamma, \quad \text{a.e. on } \Sigma, \\
\xi(\cdot, 0) &= 0 \quad \text{a.e. in } \Omega, \quad \xi_\Gamma(\cdot, 0) = 0 \quad \text{a.e. on } \Gamma. 
\end{align*}
\]

(ii) The mapping \(DS : \mathcal{U} \rightarrow L(\mathcal{X}, \mathcal{Y}), (\bar{u}, \bar{u}_\Gamma) \mapsto DS(\bar{u}, \bar{u}_\Gamma)\), satisfies for all \((\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}\) and \((h, h_\Gamma) \in \mathcal{X}\):

\[
\|DS(u, u_\Gamma) - DS(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma)\|_{\mathcal{Y}} \leq K^*_4 \|(u, u_\Gamma) - (\bar{u}, \bar{u}_\Gamma)\|_{\mathcal{H}} \|(h, h_\Gamma)\|_{\mathcal{H}}. 
\]
Remarks:

8. For any \((h, h_\Gamma) \in \mathcal{X}\) the linear system (20)–(22) is of the form (13)–(15) with zero initial conditions, hence has a unique solution in \(\mathcal{Y}\), and it holds
\[
\| (\xi, \xi_\Gamma) \|_{\mathcal{Y}} \leq \hat{C} \| (h, h_\Gamma) \|_{\mathcal{H}} .
\]
Remarks:

8. For any \((h, h_{\Gamma}) \in X\) the linear system (20)–(22) is of the form (13)–(15) with zero initial conditions, hence has a unique solution in \(Y\), and it holds
\[
\| (\zeta, \zeta_{\Gamma}) \|_Y \leq \hat{C} \| h, h_{\Gamma} \|_H.
\]

9. By Theorem 4 the reduced cost functional \(J(u, u_{\Gamma}) := J(S(u, u_{\Gamma}), (u, u_{\Gamma}))\) is Fréchet differentiable at every \((u, u_{\Gamma}) \in U\) with the derivative
\[
DJ(\bar{u}, \bar{u}_{\Gamma}) = D_{(y, y_{\Gamma})} J(S(\bar{u}, \bar{u}_{\Gamma}), (\bar{u}, \bar{u}_{\Gamma})) \circ DS(\bar{u}, \bar{u}_{\Gamma})
\]
\[
+ D_{(u, u_{\Gamma})} J(S(\bar{u}, \bar{u}_{\Gamma}), (\bar{u}, \bar{u}_{\Gamma})).
\]
Remarks:

8. For any \((h, h_\Gamma) \in \mathcal{X}\) the linear system (20)–(22) is of the form (13)–(15) with zero initial conditions, hence has a unique solution in \(\mathcal{Y}\), and it holds

\[ \| (\xi, \xi_\Gamma) \|_{\mathcal{Y}} \leq \hat{C} \| h, h_\Gamma \|_{\mathcal{H}}. \]

9. By Theorem 4 the reduced cost functional \(J(u, u_\Gamma) := J(S(u, u_\Gamma), (u, u_\Gamma))\) is Fréchet differentiable at every \((u, u_\Gamma) \in \mathcal{U}\) with the derivative

\[
D J(\bar{u}, \bar{u}_\Gamma) = D_{(y, y_\Gamma)} J(S(\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma)) \circ DS(\bar{u}, \bar{u}_\Gamma) \\
+ D_{(u, u_\Gamma)} J(S(\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma)).
\] (24)

Now notice that \(\mathcal{U}_{ad}\) is convex, hence we must have

\[
D J(\bar{u}, \bar{u}_\Gamma)(v - \bar{u}, v_\Gamma - \bar{u}_\Gamma) \geq 0 \quad \forall (v, v_\Gamma) \in \mathcal{U}_{ad}.
\] (25)

for any minimizer \((u, u_\Gamma) \in \mathcal{U}_{ad}\) of \(J\).
In terms of our cost functional, this means that the following variational inequality must be satisfied: for every \((v, v_\Gamma) \in \mathcal{U}_{ad}\) it holds

\[
\begin{align*}
&\beta_1 \int_0^T \int_\Omega (\bar{y} - z_Q) \xi \, dx \, dt + \beta_2 \int_0^T \int_\Gamma (\bar{y}_\Gamma - z_\Sigma) \zeta_\Gamma \, d\Gamma \, dt \\
&+ \beta_3 \int_\Omega (\bar{y}(\cdot, T) - z_T) \xi(\cdot, T) \, dx + \beta_4 \int_\Gamma (\bar{y}_\Gamma(\cdot, T) - z_{\Gamma,T}) \zeta_\Gamma(\cdot, T) \, d\Gamma \\
&+ \beta_5 \int_0^t \int_\Omega \bar{u}(v - \bar{u}) \, dx \, dt + \beta_6 \int_0^t \int_\Gamma \bar{u}_\Gamma(v_\Gamma - \bar{u}_\Gamma) \, d\Gamma \, dt \geq 0, 
\end{align*}
\]

where \((\xi, \zeta_\Gamma) \in \mathcal{Y}\) is the unique solution to (20)–(22) with \((h, h_\Gamma) = (v - \bar{u}, v_\Gamma - \bar{u}_\Gamma)\). We aim to eliminate \((\xi, \zeta_\Gamma)\) by introducing the adjoint state system.
First-order necessary conditions

(A6) It holds $\beta_3 = \beta_4$ and $z_{\Gamma,T} = z_T|_{\Gamma}$.

**Theorem 6:** Let the assumptions (A1)–(A6) be satisfied, and let $(\bar{u}, \bar{u}_\Gamma) \in U_{ad}$ be optimal and $(\bar{y}, \bar{y}_\Gamma) = S(\bar{u}, \bar{u}_\Gamma) \in Y$. Then the adjoint state system

\begin{align*}
- p_t - \Delta p + f'''(\bar{y}) p &= \beta_1 (\bar{y} - z_Q) \quad \text{a.e. in } Q, \tag{27} \\
\partial_n p - \partial_t p_{\Gamma} - \Delta_{\Gamma} p_{\Gamma} + g''(\bar{y}_\Gamma) p_{\Gamma} &= \beta_2 (\bar{y}_\Gamma - z_\Sigma) \quad \text{a.e. on } \Sigma, \tag{28} \\
p(\cdot, T) &= \beta_3 (\bar{y}(\cdot, T) - z_T) \quad \text{a.e. in } \Omega, \\
p_{\Gamma}(\cdot, T) &= \beta_4 (\bar{y}_\Gamma(\cdot, T) - z_{\Gamma,T}) \quad \text{a.e. on } \Gamma, \tag{29}
\end{align*}

has a unique solution $(p, p_{\Gamma}) \in Y$, and for every $(v, v_{\Gamma}) \in U_{ad}$ we have

\begin{align*}
\int_0^T \int_{\Omega} (p + \beta_5 \bar{u})(v - \bar{u}) \, dx \, dt + \int_0^T \int_{\Gamma} (p_{\Gamma} + \beta_6 \bar{u}_{\Gamma})(v_{\Gamma} - \bar{u}_{\Gamma}) \, d\Gamma \, dt \geq 0. \tag{30}
\end{align*}
First-order necessary conditions

Remarks:

10. The compatibility condition (A6) was needed to guarantee the applicability of Theorem 2 (namely, to have \( p(\cdot, T) |_\Gamma = p_\Gamma(\cdot, T) \)).

11. As usual, the Fréchet derivative \( D\mathcal{J}(\bar{u}, \bar{u}_\Gamma) \in \mathcal{L}(\mathcal{X}, \mathcal{Y}) \) can be identified with the pair \((p + \beta_5 \bar{u}, p_\Gamma + \beta_6 \bar{u}_\Gamma)\). In fact, with the standard inner product \((\cdot, \cdot)_\mathcal{H}\) in \( \mathcal{H} \) we have for all \((h, h_\Gamma) \in \mathcal{X} : \)

\[
D\mathcal{J}(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma) = ((p + \beta_5 \bar{u}, p_\Gamma + \beta_6 \bar{u}_\Gamma), (h, h_\Gamma))_\mathcal{H}.
\]

12. If \( \beta_5 > 0 \) and \( \beta_6 > 0 \), then it follows

\[
\bar{u}(x, t) = \mathbb{P}_{[\bar{u}_1(x, t), \bar{u}_2(x, t)]}(-\beta_5^{-1} p(x, t)),
\]

\[
\bar{u}_\Gamma(x, t) = \mathbb{P}_{[\bar{u}_{1\Gamma}(x, t), \bar{u}_{2\Gamma}(x, t)]}(-\beta_6^{-1} p_\Gamma(x, t))
\]

(31)

where

\[
\mathbb{P}_{[a,b]}(x) = \begin{cases} 
  a, & x < a \\
  x, & a \leq x \leq b \\
  b, & x > b 
\end{cases} \quad (32)
\]
13. The variational inequality (30) follows from (26), since it holds the identity

\[
\beta_1 \int_0^T \int_\Omega (\bar{y} - z_Q) \xi \, dx \, dt + \beta_2 \int_0^T \int_\Gamma (\bar{y}_\Gamma - z_\Sigma) \xi_\Gamma \, d\Gamma \, dt \\
+ \beta_3 \int_\Omega (\bar{y}(\cdot, T) - z_T) \xi(\cdot, T) \, dx + \beta_4 \int_\Gamma (\bar{y}_\Gamma(\cdot, T) - z_{\Gamma, T}) \xi_\Gamma(\cdot, T) \, d\Gamma
\]

\[
= \int_0^T \int_\Omega p \, h \, dx \, dt + \int_0^T \int_\Gamma p_\Gamma \, h_\Gamma \, d\Gamma \, dt,
\]

which follows from (20)–(22) and (27)–(29) using repeated integration by parts.
Concluding remarks

14. It is possible to derive second-order sufficient optimality conditions. To this end, it has to be shown that the control-to-state operator $S$ is twice continuously differentiable. This requires to assume $f, g \in C^4(0, 1)$. The second Fréchet derivative $D^2 S(\bar{u}, \bar{u}_\Gamma)$ is defined as follows: if $(h, h_\Gamma), (k, k_\Gamma) \in X$ are arbitrary then

$$D^2 S(\bar{u}, \bar{u}_\Gamma)[(h, h_\Gamma), (k, k_\Gamma)] =: (\eta, \eta_\Gamma) \in \mathcal{Y}$$

is the unique solution to the IVBP

$$\eta_t - \Delta \eta + f''(\bar{y}) \eta = -f^{(3)}(\bar{y}) \phi \psi \quad \text{a.e. in } Q,$$

$$\partial_n \eta + \partial_t \eta_\Gamma - \Delta \eta_\Gamma + g''(\bar{y}_\Gamma) \eta_\Gamma = -g^{(3)}(\bar{y}_\Gamma) \phi_\Gamma \psi_\Gamma \quad \text{a.e. on } \Sigma,$$

$$\eta(\cdot, 0) = 0 \quad \text{a.e. in } \Omega, \quad \eta_\Gamma(\cdot, 0) = 0 \quad \text{a.e. on } \Gamma,$$

where

$$(\bar{y}, \bar{y}_\Gamma) = S(\bar{u}, \bar{u}_\Gamma), \quad (\phi, \phi_\Gamma) = DS(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma),$$

$$(\psi, \psi_\Gamma) = DS(\bar{u}, \bar{u}_\Gamma)(k, k_\Gamma).$$

The proof is technical, but not too difficult (see Colli–Sprekels, WIAS-Preprint No. 1750).
Concluding remarks

It turns out that the mapping

\[ D^2 S : \mathcal{U} \to \mathcal{L}(\mathcal{X}, \mathcal{L}(\mathcal{X}, \mathcal{Y})), \quad (\bar{u}, \bar{u}_\Gamma) \mapsto D^2 S(\bar{u}, \bar{u}_\Gamma), \]

is Lipschitz continuous on \( \mathcal{U} \subset \mathcal{X} \) only in the following sense: there exists a constant \( K_5^* > 0 \) such that for every \( (u, u_\Gamma), (\bar{u}, \bar{u}_\Gamma) \in \mathcal{U} \) and all \( (h, h_\Gamma), (k, k_\Gamma) \in \mathcal{X} \) it holds

\[
\| (D^2 S(u, u_\Gamma) - D^2 S(\bar{u}, \bar{u}_\Gamma))[(h, h_\Gamma), (k, k_\Gamma)] \|_\mathcal{Y} \\
\leq K_5^* \| (u, u_\Gamma) - (\bar{u}, \bar{u}_\Gamma) \|_\mathcal{H} \| (h, h_\Gamma) \|_\mathcal{H} \| (k, k_\Gamma) \|_\mathcal{H}. \tag{37}
\]

Notice: we have to deal with a two-norm discrepancy.

15. The problem becomes considerably more difficult in the case of non-differentiability. In the paper Colli–Farshbaf-Shaker–Sprekels (in preparation), we have considered the same cost functional \( J \) (with \( \beta_3 = \beta_4 \)) and the same set of control constraints \( \mathcal{U}_{ad} \). The state system has the form:
Concluding remarks

\[ y_t - \Delta y + \zeta + f'_2(y) = u \quad \text{a.e. in } Q \]  \hfill (38)

\[ \partial_t y_{\Gamma} - \Delta_{\Gamma} y_{\Gamma} + \partial_n y + \zeta_{\Gamma} + g'_2(y_{\Gamma}) = u_{\Gamma} \quad \text{a.e. on } \Sigma \]  \hfill (39)

\[ \zeta \in \partial I_{[-1,1]}(y) \quad \text{a.e. in } Q, \quad \zeta_{\Gamma} \in \partial I_{[-1,1]}(y_{\Gamma}) \quad \text{a.e. on } \Sigma \]  \hfill (40)

\[ y(\cdot, 0) = y_0 \quad \text{a.e. in } \Omega, \quad y_{\Gamma}(\cdot, 0) = y_{0\Gamma} \quad \text{a.e. on } \Gamma. \]  \hfill (41)
Concluding remarks

\[ y_t - \Delta y + \xi + f'_2(y) = u \quad \text{a.e. in } Q \quad (38) \]
\[ \partial t y_{\Gamma} - \Delta_{\Gamma} y_{\Gamma} + \partial_n y + \xi_{\Gamma} + g'_2(y_{\Gamma}) = u_{\Gamma} \quad \text{a.e. on } \Sigma \quad (39) \]
\[ \xi \in \partial I_{[-1,1]}(y) \quad \text{a.e. in } Q, \quad \xi_{\Gamma} \in \partial I_{[-1,1]}(y) \quad \text{a.e. on } \Sigma \quad (40) \]
\[ y(\cdot, 0) = y_0 \quad \text{a.e. in } \Omega, \quad y_{\Gamma}(\cdot, 0) = y_{0\Gamma} \quad \text{a.e. on } \Gamma. \quad (41) \]

The general idea of handling this control problem was to use a deep quench approach using the results of the differentiable case: one replaces the inclusions (35) by

\[ \xi = \varphi(\alpha) h'(y), \quad \xi_{\Gamma} = \psi(\alpha) h'(y), \quad (42) \]

where \( \varphi(\alpha) = \psi(\alpha) = o(\alpha) \) as \( \alpha \downarrow 0 \) and \( 0 < \varphi(\alpha) \leq C \psi(\alpha) \) for \( \alpha > 0 \), as well as

\[ h(r) = (1 - r) \log(1 - r) + (1 + r) \log(1 + r), \quad -1 \leq r \leq +1. \quad (43) \]
Concluding remarks

This approach turns out to be successful:

■ **“Global” result:** If \( \alpha_n \downarrow 0 \) and \( (\bar{u}^{\alpha_n}, \bar{u}^{\alpha_n}_\Gamma) \) is an optimal control of the \( \alpha_n \)-approximating differentiable problem, \( n \in \mathbb{N} \), then a subsequence converges weakly to an optimal control of the non-differentiable problem.
Concluding remarks

This approach turns out to be successful:

■ **“Global” result:** If $\alpha_n \downarrow 0$ and $(\bar{u}^{\alpha_n}, \bar{u}^\alpha_{\Gamma})$ is an optimal control of the $\alpha_n$-approximating differentiable problem, $n \in \mathbb{N}$, then a subsequence converges weakly to an optimal control of the non-differentiable problem.

■ **“Local” result:** For any fixed optimizer $(\bar{u}, \bar{u}_{\Gamma})$ define the “adapted” cost functional

$$\tilde{J}((y, y_{\Gamma}), (u, u_{\Gamma})) = J((y, y_{\Gamma}), (u, u_{\Gamma})) + \frac{1}{2} ||u - \bar{u}||_{L^2(Q)}^2 + \frac{1}{2} ||u_{\Gamma} - \bar{u}_{\Gamma}||^2.$$

Then consider the $\alpha$-approximating problems with this functional. It holds:
Concluding remarks

This approach turns out to be successful:

■ **“Global” result:** If $\alpha_n \downarrow 0$ and $(\bar{u}^{\alpha_n}, \bar{u}^{\alpha_n}_\Gamma)$ is an optimal control of the $\alpha_n$-approximating differentiable problem, $n \in \mathbb{N}$, then a subsequence converges weakly to an optimal control of the non-differentiable problem.

■ **“Local” result:** For any fixed optimizer $(\bar{u}, \bar{u}_\Gamma)$ define the “adapted” cost functional

$$\tilde{J}((y, y_\Gamma), (u, u_\Gamma)) = J((y, y_\Gamma), (u, u_\Gamma)) + \frac{1}{2} \|u - \bar{u}\|_{L^2(Q)}^2 + \frac{1}{2} \|u_\Gamma - \bar{u}_\Gamma\|^2.$$  

Then consider the $\alpha$-approximating problems with this functional. It holds:

- $\exists \alpha_n \downarrow 0$ and minimizers $(\bar{u}^{\alpha_n}, \bar{u}^{\alpha_n}_\Gamma)$ of the $\alpha_n$-approximating problems such that $(\bar{u}^{\alpha_n}, \bar{u}^{\alpha_n}_\Gamma) \rightarrow (\bar{u}, \bar{u}_\Gamma)$ strongly in $\mathcal{H}$. 

Concluding remarks

This approach turns out to be successful:

■ **“Global” result:** If $\alpha_n \downarrow 0$ and $(\bar{u}_\alpha^n, \bar{u}_\Gamma^n)$ is an optimal control of the $\alpha_n$-approximating differentiable problem, $n \in \mathbb{N}$, then a subsequence converges weakly to an optimal control of the non-differentiable problem.

■ **“Local” result:** For any fixed optimizer $(\bar{u}, \bar{u}_\Gamma)$ define the “adapted” cost functional

$$\tilde{J}((y, y_\Gamma), (u, u_\Gamma)) = J((y, y_\Gamma), (u, u_\Gamma)) + \frac{1}{2} \|u - \bar{u}\|^2_{L^2(Q)} + \frac{1}{2} \|u_\Gamma - \bar{u}_\Gamma\|^2.$$

Then consider the $\alpha$-approximating problems with this functional. It holds:

- $\exists \alpha_n \downarrow 0$ and minimizers $(\bar{u}_\alpha^n, \bar{u}_\Gamma^n)$ of the $\alpha_n$-approximating problems such that $(\bar{u}_\alpha^n, \bar{u}_\Gamma^n) \rightarrow (\bar{u}, \bar{u}_\Gamma)$ strongly in $\mathcal{H}$.

- Letting $\alpha_n \downarrow 0$ in the first-order necessary optimality conditions for the $\alpha_n$-approximating problems leads to first-order conditions for the non-differentiable case.

