



Weierstrass Institute for
Applied Analysis and Stochastics



Optimal control of phase field systems involving dynamic boundary conditions and singular nonlinearities

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(joint work with P. Colli, G. Gilardi (Pavia), M. H. Farshbaf-Shaker (WIAS))

Consider the IVP with dynamic boundary condition

$$y_t - \Delta y + f'(y) = u \quad \text{a.e. in } Q, \quad (1)$$

$$\partial_t y_\Gamma - \Delta_\Gamma y_\Gamma + \partial_n y + g'(y_\Gamma) = u_\Gamma, \quad y|_\Gamma = y_\Gamma, \quad \text{a.e. on } \Sigma, \quad (2)$$

$$y(0) = y_0 \quad \text{a.e. in } \Omega, \quad y_\Gamma(0) = y_{0_\Gamma} \quad \text{a.e. on } \Gamma. \quad (3)$$

Here, we have

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

The system (1)–(3) constitutes a model for an isothermal phase transition between two different phases that takes place in the container $\Omega \subset \mathbb{R}^3$ and is accompanied by surface diffusion on the boundary Γ . Here, y plays the role of a **non-conserved** “order parameter” (Allen–Cahn type) of the phase transition, which is typically the fraction of one of the phases and therefore should attain values in $[0, 1]$.

The corresponding “free energy” is of the form

$$\mathcal{F}(y) = \int_{\Omega} \left(f(y) + \frac{1}{2} |\nabla y|^2 \right) dx + \int_{\Gamma} \left(g(y_{\Gamma}) + \frac{1}{2} |\nabla_{\Gamma} y_{\Gamma}|^2 \right) d\Gamma,$$

where ∇_{Γ} denotes the surface gradient.

We remark that the corresponding system for a **conserved** order parameter (Cahn–Hilliard type) can also be treated, but is more difficult.

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

$$z_Q \in L^2(Q), \quad z_\Sigma \in L^2(\Sigma), \quad z_T \in V, \quad z_{\Gamma, T} \in V_\Gamma,$$

$$\tilde{u}_1, \tilde{u}_2 \in L^\infty(Q) \text{ with } \tilde{u}_1 \leq \tilde{u}_2 \text{ a.e. in } Q,$$

$$\tilde{u}_{1\Gamma}, \tilde{u}_{2\Gamma} \in L^\infty(\Sigma) \text{ with } \tilde{u}_{1\Gamma} \leq \tilde{u}_{2\Gamma} \text{ a.e. on } \Sigma.$$

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

$$\begin{aligned}
 J((y, y_\Gamma), (u, u_\Gamma)) &:= \frac{\beta_1}{2} \iint_{0\Omega}^T |y - z_Q|^2 \, dx \, dt + \frac{\beta_2}{2} \iint_{0\Gamma}^T |y_\Gamma - z_\Sigma|^2 \, d\Gamma \, dt \\
 &+ \frac{\beta_3}{2} \int_{\Omega} |y(\cdot, T) - z_T|^2 \, dx + \frac{\beta_4}{2} \int_{\Gamma} |y_\Gamma(\cdot, T) - z_{\Gamma,T}|^2 \, d\Gamma \\
 &+ \frac{\beta_5}{2} \iint_{0\Omega}^T |u|^2 \, dx \, dt + \frac{\beta_6}{2} \iint_{0\Gamma}^T |u_\Gamma|^2 \, d\Gamma \, dt
 \end{aligned} \tag{4}$$

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

$$\begin{aligned}
 (u, u_\Gamma) \in \mathcal{U}_{\text{ad}} &:= \{(w, w_\Gamma) \in \mathcal{H} : \tilde{u}_1 \leq w \leq \tilde{u}_2 \text{ a.e. in } Q, \\
 &\tilde{u}_{1\Gamma} \leq w_\Gamma \leq \tilde{u}_{2\Gamma} \text{ a.e. on } \Sigma \}.
 \end{aligned} \tag{5}$$

(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:

$$\lim_{r \searrow 0} f_1'(r) = \lim_{r \searrow 0} g_1'(r) = -\infty, \quad \lim_{r \nearrow 1} f_1'(r) = \lim_{r \nearrow 1} g_1'(r) = +\infty \quad (6)$$

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

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(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

$$0 < y_0 < 1 \quad \text{a.e. in } \Omega, \quad 0 < y_{0\Gamma} < 1 \quad \text{a.e. on } \Gamma. \quad (8)$$

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$$0 < y_0 < 1 \quad \text{a.e. in } \Omega, \quad 0 < y_{0\Gamma} < 1 \quad \text{a.e. on } \Gamma. \quad (8)$$

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

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

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 $c_1 > 0, c_2 > 0$.

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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 was studied in Colli–Farshbaf–Shaker–Sprekels (to appear 2014 in Appl. Math. Optim.): 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 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 $(u, u_\Gamma) \in \mathcal{H}$ a unique solution $(y, y_\Gamma) \in \mathcal{Y}$ such that

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

(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

$$\|(y, y_\Gamma)\|_{\mathcal{Y}} \leq K_1^*, \quad \|f'(y)\|_{L^2(Q)} + \|g'(y_\Gamma)\|_{L^2(\Sigma)} \leq K_1^*. \quad (11)$$

Moreover, $\exists K_2^* > 0$: whenever $(u_1, u_{1\Gamma}), (u_2, u_{2\Gamma}) \in \mathcal{U}$ are given, then we have

$$\begin{aligned} & \|y_1 - y_2\|_{C^0([0,T];H)} + \|\nabla(y_1 - y_2)\|_{L^2(Q)} + \|y_{1\Gamma} - y_{2\Gamma}\|_{C^0([0,T];H_\Gamma)} \\ & + \|\nabla_\Gamma(y_{1\Gamma} - y_{2\Gamma})\|_{L^2(\Sigma)} \\ & \leq K_2^* \left(\|u_1 - u_2\|_{L^2(Q)} + \|u_{1\Gamma} - u_{2\Gamma}\|_{L^2(\Sigma)} \right). \end{aligned} \quad (12)$$

Remark:

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

$$\mathcal{S} : (u, u_\Gamma) \mapsto \mathcal{S}(u, u_\Gamma) := (y, y_\Gamma)$$

is defined as a mapping from \mathcal{X} into \mathcal{Y} . Moreover, \mathcal{S} is Lipschitz continuous when viewed as a mapping from the subset \mathcal{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 $(w_0, w_{0\Gamma}) \in V \times V_\Gamma$ with $w_{0\Gamma} = w_{0\Gamma}$ be given. Then we have:

(i) The linear IBVP

$$w_t - \Delta w + c_1(x, t) w = u \quad \text{a.e. in } Q, \quad (13)$$

$$\partial_t w_\Gamma - \Delta_\Gamma w_\Gamma + \partial_n w + c_2(x, t) w_\Gamma = u_\Gamma, \quad w|_\Gamma = w_\Gamma, \quad \text{a.e. on } \Sigma, \quad (14)$$

$$w(\cdot, 0) = w_0 \quad \text{a.e. in } \Omega, \quad w_\Gamma(\cdot, 0) = w_{0\Gamma} \quad \text{a.e. on } \Gamma, \quad (15)$$

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

$$\|(w, w_\Gamma)\|_{\mathcal{Y}} \leq \hat{C} \|(u, u_\Gamma)\|_{\mathcal{H}}. \quad (16)$$

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

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

Comparison in (13) yields

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

Then, applying a standard embedding result,

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

whence, by the trace theorem,

$$\|\partial_n w\|_{L^2(0,T;H_\Gamma)} \leq C_4 \|(u, u_\Gamma)\|_{\mathcal{H}}.$$

But then, by comparison in (14),

$$\|\Delta_{\Gamma} w_{\Gamma}\|_{L^2(\Sigma)} \leq C_5 \|(u, u_{\Gamma})\|_{\mathcal{H}},$$

whence

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

Standard elliptic estimates then yield

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



Remark:

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

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

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

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

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

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

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

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

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Remark:

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

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

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

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

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

$$r^* \geq \max \left\{ \operatorname{ess\,sup}_{x \in \Omega} y_0(x), \operatorname{ess\,sup}_{x \in \Gamma} y_{0_\Gamma}(x) \right\},$$

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

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

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

$$\begin{aligned} 0 &= \frac{1}{2} \|w(T)\|_H^2 + \int_0^T \|\nabla w(t)\|_H^2 dt + \int_0^T \|\nabla_\Gamma w_\Gamma(t)\|_{H_\Gamma}^2 dt \\ &\quad + \frac{1}{2} \|w_\Gamma(T)\|_{H_\Gamma}^2 + \Phi, \end{aligned}$$

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

$$\|(y_1, y_{1\Gamma}) - (y_2, y_{2\Gamma})\|_{\mathcal{Y}} \leq K_3^* \|(u_1, u_{1\Gamma}) - (u_2, u_{2\Gamma})\|_{\mathcal{H}}. \quad (19)$$

This higher Lipschitz continuity is needed to show the Fréchet differentiability of the control-to-state mapping \mathcal{S} .

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

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

Proof: Pick a minimizing sequence $\{(u_n, u_{n\Gamma})\} \subset \mathcal{U}_{\text{ad}}$, and let

$(u_n, u_{n\Gamma}) = \mathcal{S}(u_n, u_{n\Gamma})$, $n \in \mathbb{N}$. By the a priori estimates, we may assume that

$$u_n \rightharpoonup \bar{u} \text{ weakly-}^* \text{ in } L^\infty(Q), \quad u_{n\Gamma} \rightharpoonup \bar{u}_\Gamma \text{ weakly-}^* \text{ in } L^\infty(\Sigma),$$

$$y_n \rightharpoonup \bar{y} \text{ weakly-}^* \text{ in } H^1(0, T; H) \cap L^\infty(0, T; V) \cap L^2(0, T; H^2(\Omega)) \cap L^\infty(Q),$$

$$y_{n\Gamma} \rightharpoonup \bar{y}_\Gamma \text{ weakly-}^* \text{ in } H^1(0, T; H_\Gamma) \cap L^\infty(0, T; V_\Gamma) \cap L^2(0, T; H^2(\Gamma)) \cap L^\infty(\Sigma).$$

In particular, we have (by compact embedding)

$$y_n \rightarrow \bar{y} \text{ strongly in } C^0([0, T]; H), \quad y_{n\Gamma} \rightarrow \bar{y}_\Gamma \text{ strongly in } C^0([0, T]; H_\Gamma).$$

Passage to the limit $n \rightarrow \infty$ in (1)–(3) easily shows that $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}, \bar{u}_\Gamma)$, 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 $\mathcal{S} : \mathcal{X} \rightarrow \mathcal{Y}$ is Fréchet differentiable at $(\bar{u}, \bar{u}_\Gamma)$, and the Fréchet derivative $D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)$ is given by $D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma) = (\zeta, \zeta_\Gamma)$, where for any given $(h, h_\Gamma) \in \mathcal{X}$ the pair $(\zeta, \zeta_\Gamma) \in \mathcal{Y}$ solves the linearized system

$$\zeta_t - \Delta \zeta + f''(\bar{y}) \zeta = h \quad \text{a.e. in } Q, \quad (20)$$

$$\partial_t \zeta_\Gamma - \Delta_\Gamma \zeta_\Gamma + \partial_n \zeta + g''(\bar{y}_\Gamma) \zeta_\Gamma = h_\Gamma, \quad \zeta_\Gamma = \zeta|_\Gamma, \quad \text{a.e. on } \Sigma, \quad (21)$$

$$\zeta(\cdot, 0) = 0 \quad \text{a.e. in } \Omega, \quad \zeta_\Gamma(\cdot, 0) = 0 \quad \text{a.e. on } \Gamma. \quad (22)$$

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

$$\|(D\mathcal{S}(u, u_\Gamma) - D\mathcal{S}(\bar{u}, \bar{u}_\Gamma))(h, h_\Gamma)\|_{\mathcal{Y}} \leq K_4^* \|(u, u_\Gamma) - (\bar{u}, \bar{u}_\Gamma)\|_{\mathcal{H}} \|(h, h_\Gamma)\|_{\mathcal{H}}. \quad (23)$$

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

$$\|(\xi, \xi_\Gamma)\|_{\mathcal{Y}} \leq \widehat{C} \|h, h_\Gamma\|_{\mathcal{H}}.$$

Remarks:

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

$$\begin{aligned} D\mathcal{J}(\bar{u}, \bar{u}_\Gamma) &= D_{(y, y_\Gamma)} J(\mathcal{S}(\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma)) \circ D\mathcal{S}(\bar{u}, \bar{u}_\Gamma) \\ &\quad + D_{(u, u_\Gamma)} J(\mathcal{S}(\bar{u}, \bar{u}_\Gamma), (\bar{u}, \bar{u}_\Gamma)). \end{aligned} \quad (24)$$

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

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

for any minimizer $(u, u_\Gamma) \in \mathcal{U}_{\text{ad}}$ of \mathcal{J} .

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

$$\begin{aligned}
 & \beta_1 \int_0^T \int_{\Omega} (\bar{y} - z_Q) \zeta \, dx \, dt + \beta_2 \int_0^T \int_{\Gamma} (\bar{y}_\Gamma - z_\Sigma) \zeta_\Gamma \, d\Gamma \, dt \\
 & + \beta_3 \int_{\Omega} (\bar{y}(\cdot, T) - z_T) \zeta(\cdot, T) \, dx + \beta_4 \int_{\Gamma} (\bar{y}_\Gamma(\cdot, T) - z_{\Gamma, T}) \zeta_\Gamma(\cdot, T) \, d\Gamma \\
 & + \beta_5 \int_0^t \int_{\Omega} \bar{u}(v - \bar{u}) \, dx \, dt + \beta_6 \int_0^t \int_{\Gamma} \bar{u}_\Gamma(v_\Gamma - \bar{u}_\Gamma) \, d\Gamma \, dt \geq 0, \tag{26}
 \end{aligned}$$

where $(\zeta, \zeta_\Gamma) \in \mathcal{Y}$ is the unique solution to (20)–(22) with

$(h, h_\Gamma) = (v - \bar{u}, v_\Gamma - \bar{u}_\Gamma)$. We aim to eliminate (ζ, ζ_Γ) by introducing the adjoint state system.

(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 $(\bar{u}, \bar{u}_\Gamma) \in \mathcal{U}_{\text{ad}}$ be optimal and $(\bar{y}, \bar{y}_\Gamma) = \mathcal{S}(\bar{u}, \bar{u}_\Gamma) \in \mathcal{Y}$. Then the adjoint state system

$$-p_t - \Delta p + f''(\bar{y}) p = \beta_1 (\bar{y} - z_Q) \quad \text{a.e. in } Q, \quad (27)$$

$$\partial_n p - \partial_t p_\Gamma - \Delta_\Gamma p_\Gamma + g''(\bar{y}_\Gamma) p_\Gamma = \beta_2 (\bar{y}_\Gamma - z_\Sigma) \quad \text{a.e. on } \Sigma, \quad (28)$$

$$p(\cdot, T) = \beta_3 (\bar{y}(\cdot, T) - z_T) \quad \text{a.e. in } \Omega,$$

$$p_\Gamma(\cdot, T) = \beta_4 (\bar{y}_\Gamma(\cdot, T) - z_{\Gamma,T}) \quad \text{a.e. on } \Gamma, \quad (29)$$

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

$$\int_0^T \int_\Omega (p + \beta_5 \bar{u})(v - \bar{u}) \, dx \, dt + \int_0^T \int_\Gamma (p_\Gamma + \beta_6 \bar{u}_\Gamma)(v_\Gamma - \bar{u}_\Gamma) \, d\Gamma \, dt \geq 0. \quad (30)$$

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

$$\begin{aligned} \bar{u}(x, t) &= \mathbb{P}_{[\bar{u}_1(x, t), \bar{u}_2(x, t)]}(-\beta_5^{-1} p(x, t)), \\ \bar{u}_{\Gamma}(x, t) &= \mathbb{P}_{[\bar{u}_{1\Gamma}(x, t), \bar{u}_{2\Gamma}(x, t)]}(-\beta_6^{-1} p_{\Gamma}(x, t)) \end{aligned} \quad (31)$$

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

$$\begin{aligned} & \beta_1 \int_0^T \int_{\Omega} (\bar{y} - z_Q) \xi \, dx \, dt + \beta_2 \int_0^T \int_{\Gamma} (\bar{y}_{\Gamma} - z_{\Sigma}) \xi_{\Gamma} \, d\Gamma \, dt \\ & + \beta_3 \int_{\Omega} (\bar{y}(\cdot, T) - z_T) \xi(\cdot, T) \, dx + \beta_4 \int_{\Gamma} (\bar{y}_{\Gamma}(\cdot, T) - z_{\Gamma, T}) \xi_{\Gamma}(\cdot, T) \, d\Gamma \\ & = \int_0^T \int_{\Omega} p h \, dx \, dt + \int_0^T \int_{\Gamma} p_{\Gamma} h_{\Gamma} \, d\Gamma \, dt, \end{aligned}$$

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

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 \mathcal{S} is **twice continuously differentiable**. This requires to assume $f, g \in C^4(0, 1)$. The second Fréchet derivative $D^2\mathcal{S}(\bar{u}, \bar{u}_\Gamma)$ is defined as follows: if $(h, h_\Gamma), (k, k_\Gamma) \in \mathcal{X}$ are arbitrary then

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

is the unique solution to the IVBP

$$\eta_t - \Delta\eta + f''(\bar{y})\eta = -f^{(3)}(\bar{y})\phi\psi \quad \text{a.e. in } Q, \quad (33)$$

$$\partial_n\eta + \partial_t\eta_\Gamma - \Delta_\Gamma\eta_\Gamma + g''(\bar{y}_\Gamma)\eta_\Gamma = -g^{(3)}(\bar{y}_\Gamma)\phi_\Gamma\psi_\Gamma \quad \text{a.e. on } \Sigma, \quad (34)$$

$$\eta(\cdot, 0) = 0 \quad \text{a.e. in } \Omega, \quad \eta_\Gamma(\cdot, 0) = 0 \quad \text{a.e. on } \Gamma, \quad (35)$$

where

$$\begin{aligned} (\bar{y}, \bar{y}_\Gamma) &= \mathcal{S}(\bar{u}, \bar{u}_\Gamma), & (\phi, \phi_\Gamma) &= D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)(h, h_\Gamma), \\ (\psi, \psi_\Gamma) &= D\mathcal{S}(\bar{u}, \bar{u}_\Gamma)(k, k_\Gamma). \end{aligned} \quad (36)$$

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

It turns out that the mapping

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

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

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

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

15. The problem is considerably more difficult in the case of non-differentiability. In the paper Colli–Farshbaf–Shaker–Sprekels (to appear in Appl. Math. Optim.), we 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:

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

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

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

$$y(\cdot, 0) = y_0 \quad \text{a.e. in } \Omega, \quad y_\Gamma(\cdot, 0) = y_{0_\Gamma} \quad \text{a.e. on } \Gamma. \quad (41)$$

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$$\xi \in \partial I_{[-1,1]}(y) \quad \text{a.e. in } Q, \quad \xi_\Gamma \in \partial I_{[-1,1]}(y) \quad \text{a.e. on } \Sigma \quad (40)$$

$$y(\cdot, 0) = y_0 \quad \text{a.e. in } \Omega, \quad y_\Gamma(\cdot, 0) = y_{0\Gamma} \quad \text{a.e. on } \Gamma. \quad (41)$$

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 $\alpha \searrow 0$ and $0 < \varphi(\alpha) \leq C\psi(\alpha)$ for $\alpha > 0$, as well as

$$h(r) = (1 - r) \log(1 - r) + (1 + r) \log(1 + r), \quad -1 \leq r \leq +1. \quad (43)$$

This approach turns out to be successful:

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

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- **“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 α -approximating problems with this functional. It holds:

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Then consider the α -approximating problems with this functional. It holds:

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

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

1. P. Colli, J. S.: *Optimal control of the Allen–Cahn equation with singular potentials and dynamic boundary condition*. WIAS Preprint No. 1750 (2012). Submitted.
2. P. Colli, M. H. Farshbaf-Shaker, J. S.: *A deep quench approach to the optimal control of an Allen–Cahn equation with dynamic boundary condition and double obstacle potentials*. WIAS Preprint No. 1838 (2013). To appear 2014 in *Appl. Math. Optim.*

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Corresponding results for the Cahn–Hilliard system (conserved case):

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