



**Weierstrass Institute for
Applied Analysis and Stochastics**



Choosing the velocity as control in a nonlocal convective Cahn-Hilliard equation

Elisabetta Rocca – with Jürgen Sprekels (WIAS) – arXiv:1404.1765v2, SIAM J. Control Optim. to appear

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(CP) Minimize the cost functional

$$J(\varphi, \mathbf{v}) = \frac{\beta_1}{2} \int_0^T \int_{\Omega} |\varphi - \varphi_Q|^2 dx dt + \frac{\beta_2}{2} \int_{\Omega} |\varphi(T) - \varphi_{\Omega}|^2 dx + \frac{\beta_3}{2} \int_0^T \int_{\Omega} |\mathbf{v}|^2 dx dt$$

subject to the *state system*

$$\varphi_t - \operatorname{div}(m(\varphi)\nabla\mu) = -\mathbf{v} \cdot \nabla\varphi \quad \text{in } Q := \Omega \times (0, T) \quad (\mathbf{P1})$$

$$\mu = f'(\varphi) + w \quad \text{in } Q \quad (\mathbf{P2})$$

$$w(x, t) = \int_{\Omega} k(|x - y|)(1 - 2\varphi(y, t)) dy \quad \text{in } Q \quad (\mathbf{P3})$$

$$m(\varphi)\nabla\mu \cdot \mathbf{n} = 0 \quad \text{on } \Sigma := \partial\Omega \times (0, T), \quad \varphi(0) = \varphi_0 \quad \text{in } \Omega \subset \mathbb{R}^3 \quad (\mathbf{P4})$$

and to the constraint that the **control** velocity \mathbf{v} belongs to a suitable closed, bounded and convex subset of the space

$$\mathcal{V} := \{\mathbf{v} \in L^2(0, T; H_{div}^1(\Omega)) \cap L^\infty(Q)^3 : \exists \mathbf{v}_t \in L^2(0, T; L^3(\Omega)^3)\}$$

where $H_{div}^1(\Omega) := \{\mathbf{v} \in H_0^1(\Omega)^3 : \operatorname{div}(\mathbf{v}) = 0\}$

- The state system:
 - nonlocal vs local
 - the nonlinearities: mobility and mixing potential

- The control problem: the choice of the velocity as control

- Well-posedness and stability

- First order necessary conditions

- Open related problems

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- (in the nonlocal case, cf. [Gajewski, Zacharias, '03], ..., [Colli, Frigeri, Grasselli, '12])

$$E(\varphi) = \frac{1}{4} \int_{\Omega} \int_{\Omega} J(x-y) (\varphi(x) - \varphi(y))^2 dx dy + \int_{\Omega} \eta f(\varphi(x)) dx$$

- $J : \mathbb{R}^d \rightarrow \mathbb{R}$ is a smooth even function, e.g. $J(x) = j_3 |x|^{-1}$ in 3D and $J(x) = -j_2 \log |x|$ in 2D
- it is justified as a macroscopic limit of microscopic phase segregation models with particle conserving dynamics (cf. [Giacomin Lebowitz, '97&'98])

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$$\int_{\Omega} n^{d+2} J(|n(x - y)|^2) |\varphi(x) - \varphi(y)|^2 dy = \int_{\Omega_n(x)} J(|z|^2) \left| \frac{\varphi(x + \frac{z}{n}) - \varphi(x)}{\frac{1}{n}} \right|^2 dz$$

$$\xrightarrow{n \rightarrow \infty} \int_{\mathbb{R}^d} J(|z|^2) \langle \nabla \varphi(x), z \rangle^2 dz = \frac{\sigma}{2} |\nabla \varphi(x)|^2$$

where we denote

- $\sigma = 2/d \int_{\mathbb{R}^d} J(|z|^2) |z|^2 dz$ and $\Omega_n(x) = n(\Omega - x)$ and we have used the identity
- $\int_{\mathbb{R}^d} J(|z|^2) \langle e, z \rangle^2 dz = 1/d \int_{\mathbb{R}^d} J(|z|^2) |z|^2 dz$ for every unit vector $e \in \mathbb{R}^d$

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A philosophical question: is diffusion local or nonlocal?

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If we consider

$$\Delta u = \lim_{\epsilon \rightarrow 0} \frac{c_\epsilon}{|B_\epsilon(x)|} \int_{B_\epsilon(x)} (u(y) - u(x)) dy,$$

the density at the point x compares itself with its values in a tiny surrounding ball. The difference between the surrounding average and the value at x , properly scaled is the “Laplacian”.

If the set to which u compares itself is not shrunk to zero, the process is an integral diffusion.

$$Lu(x) = \int J(x, y)(u(y) - u(x)) dy.”$$

The singular potential f is taken in the typical logarithmic form:

$$f(\varphi) = \varphi \log(\varphi) + (1 - \varphi) \log(1 - \varphi)$$

and the mobility m , which degenerates at the pure phases $\varphi = 0$ and $\varphi = 1$:

$$m(\varphi) = \frac{c_0}{f''(\varphi)} = c_0 \varphi(1 - \varphi) \quad \text{with some constant } c_0 > 0$$

which entails that we have the relations

$$m(\varphi) f''(\varphi) \equiv c_0, \quad m(\varphi) \nabla \mu = c_0 \nabla \varphi + m(\varphi) \nabla w$$

and the nonlocal CH-equation $\varphi_t - \operatorname{div}(m(\varphi) \nabla \mu) = -\mathbf{v} \cdot \nabla \varphi$ becomes

$$\varphi_t - c_0 \Delta \varphi - \operatorname{div} \left(m(\varphi) \nabla \left(\int_{\Omega} k(|x - y|) (1 - 2\varphi(y, t)) \, dy \right) \right) = -\mathbf{v} \cdot \nabla \varphi$$

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Actually, we could consider the more general case when

$f \in C^4(0, 1)$ is strictly convex in $(0, 1)$, $Im(f')^{-1} = [0, 1]$, $\frac{1}{f''}$ is strictly concave in $(0, 1)$

$m \in C^2([0, 1])$ satisfies $m(\varphi)f''(\varphi) \geq c_0 > 0$ for every $\varphi \in [0, 1]$

Assume that

$$(H1) \quad \int_{\Omega} \int_{\Omega} k(|x-y|) dx dy =: k_0 < +\infty, \quad \sup_{x \in \Omega} \int_{\Omega} |k(|x-y|)| dy =: \bar{k} < +\infty$$

$$(H2) \quad \forall p \in [1, +\infty] \exists k_p > 0 : \left\| -2 \int_{\Omega} k(|x-y|) z(y) dy \right\|_{W^{1,p}(\Omega)} \leq k_p \|z\|_{L^p(\Omega)}$$

for all $z \in W^{1,p}(\Omega)$

(H3) For $p \in \{2, 3\}$ there is some $s_p > 0$ such that for all $z \in W^{1,p}(\Omega)$ it holds

$$\left\| -2 \int_{\Omega} k(|x-y|) z(y) dy \right\|_{W^{2,p}(\Omega)} \leq s_p \|z\|_{W^{1,p}(\Omega)}$$

Examples:

- the classical Newton potential:

$$k(x) = \kappa |x|^{-1}, \quad x \neq 0, \quad \text{where } \kappa > 0 \text{ is a constant}$$

- the usual mollifiers, and the Gaussian kernels:

$$k(x) = \kappa_2 \exp(-|x|^2/\kappa_3), \quad x \in \mathbb{R}^3, \quad \text{where } \kappa_2 > 0 \text{ and } \kappa_3 \text{ are constants}$$

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- [ZHAO, LIU, '13, '14]: the convective 1D case and the 2D case, where the boundary conditions $\varphi = \Delta\varphi = 0$ were prescribed in place of the usual no-flux conditions for φ and the chemical potential. Notice that in all of the abovementioned contributions a distributed control was assumed which was not related to the fluid velocity

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Optimal control problems for certain classes of PDEs coupled with *nonlocal boundary conditions*: [Druet, Klein, Sprekels, Tröltzsch, and Yousept, '11], [Philip, '10], [Meyer, Yousept, '09], [Meyer, Philip, Tröltzsch, '06]

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!!! no analytical contribution on optimal control problems for nonlocal phase field models of convective Cahn-Hilliard type and, more generally, for nonlocal PDEs not on the boundary

Novelty: the use of the fluid velocity field as the control parameter \implies through the convective term there arises a nonlinear coupling between control and state in product form that renders the analysis difficult \implies the choice of the regular space for velocities is justified

Applications: growth of bulk semiconductor crystals, e.g., the block solidification of large silicon crystals for photovoltaic applications.

In this industrial process a mixture of several species of atoms (impurities) dissolved in the silicon melt has to be moved by the flow (i.e., by the velocity field \mathbf{v}) to the boundary of the solidifying silicon in order to maximize the purified high quality part of the resulting silicon ingot. In other words, the flow pattern acts as a control to optimize the final distribution of the impurities.

$$\begin{aligned}
 \text{(H4)} \quad \mathcal{V}_{\text{ad}} := \{ \mathbf{v} = (v_1, v_2, v_3) \in \mathcal{V} : & \tilde{v}_{1_i} \leq v_i \leq \tilde{v}_{2_i} \text{ a.e. in } Q, \quad i = 1, 2, 3, \\
 & \|\mathbf{v}\|_{L^2(0,T;H_{div}^1(\Omega)^3)} + \|\mathbf{v}_t\|_{L^2(0,T;L^3(\Omega)^3)} \leq V \}
 \end{aligned}$$

where $V > 0$ is a given constant and $\tilde{v}_{1_i}, \tilde{v}_{2_i} \in L^\infty(Q)$, $i = 1, 2, 3$, are given threshold functions; we generally assume that $\mathcal{V}_{\text{ad}} \neq \emptyset$.

Observe that \mathcal{V}_{ad} is a bounded, closed, and convex subset of \mathcal{V} , which is certainly contained in some bounded open subset of \mathcal{V} . For convenience, we fix such a set once and for all, noting that any other such set could be used instead:

$$\text{(H5)} \quad \mathcal{V}_R \subset \mathcal{V} \text{ is an open set satisfying } \mathcal{V}_{\text{ad}} \subset \mathcal{V}_R \text{ such that, for all } \mathbf{v} \in \mathcal{V}_R,$$

$$\|\mathbf{v}\|_{L^2(0,T;H^1(\Omega)^3)} + \|\mathbf{v}\|_{L^\infty(Q)^3} + \|\mathbf{v}_t\|_{L^2(0,T;L^3(\Omega)^3)} \leq R$$

Assume **(H1)–(H5)** and $\varphi_0 \in H^2(\Omega)$ be such that there is some $\kappa_0 > 0$ such that $0 < \kappa_0 \leq \varphi_0 \leq 1 - \kappa_0 < 1$ a.e. in Ω , and it holds a.e. in Ω that

$$\begin{aligned} 0 &= \left(c_0 \nabla \varphi_0 + m(\varphi_0) \nabla \int_{\Omega} k(|x-y|)(1-2\varphi_0(y)) dy \right) \cdot \mathbf{n} \\ &= m(\varphi_0) \nabla \mu(\cdot, 0) \cdot \mathbf{n}. \end{aligned}$$

Then, the system **(P1)–(P4)** for any $\mathbf{v} \in \mathcal{V}_R$ a unique solution triple (φ, w, μ) such that

$$\varphi \in C^1([0, T]; L^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^2(\Omega)) \cap C^0(\overline{Q}).$$

Moreover, there is $\kappa \in (0, 1)$, which does not depend on the choice of $\mathbf{v} \in \mathcal{V}_R$, such that

$$0 < \kappa \leq \varphi \leq 1 - \kappa < 1 \quad \text{a.e. in } Q.$$

Finally, there exists a constant $K_2^* > 0$, which only depends on the data of the state system and on R , such that it holds:

$$\begin{aligned} \int_0^t \|(\varphi_1 - \varphi_2)_t(s)\|_{L^2(\Omega)}^2 ds + \max_{0 \leq s \leq t} \|(\varphi_1 - \varphi_2)(s)\|_{H^1(\Omega)}^2 \leq \\ K_2^* \int_0^t \|(\mathbf{v}_1 - \mathbf{v}_2)(s)\|_{L^3(\Omega)^3}^2 ds \end{aligned}$$

Owing to the previous results, the *control-to-state operator*

$$\begin{aligned} \mathcal{S} : \mathcal{V}_R &\rightarrow C^1([0, T]; L^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^2(\Omega)) \\ \mathbf{v} &\mapsto \varphi \end{aligned}$$

is well defined and Lipschitz continuous as a mapping from \mathcal{V}_R (viewed as a subset of $L^2(0, T; L^3(\Omega)^3)$) into $H^1(0, T; L^2(\Omega)) \cap C^0([0, T]; H^1(\Omega))$.

Then we have the first result:

Theorem 1. Suppose that the previous hypotheses are fulfilled. Then the problem (CP) admits a solution $\bar{\mathbf{v}} \in \mathcal{V}_{ad}$

Assume that $\bar{\mathbf{v}} \in \mathcal{V}_R$ is fixed and that $(\bar{\varphi}, \bar{w}, \bar{\mu})$ is the associated triple solving the state system, i.e., $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$, $\bar{w} = \mathcal{K}(\bar{\varphi})$, $\bar{\mu} = f'(\bar{\varphi}) + \bar{w}$.

Suppose that an arbitrary $\mathbf{h} \in \mathcal{V}$ is given.

Consider the linearized system obtained by linearizing the state system at $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$:

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Suppose that an arbitrary $\mathbf{h} \in \mathcal{V}$ is given.

Consider the linearized system obtained by linearizing the state system at $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$:

$$\begin{aligned} \xi_t - c_0 \Delta \xi - \operatorname{div} \left(m'(\bar{\varphi}) \xi \nabla \bar{w} - 2 m(\bar{\varphi}) \nabla \left(\int_{\Omega} k(|x-y|) \xi(y, \cdot) dy \right) \right) \\ = -\mathbf{h} \cdot \nabla \bar{\varphi} - \bar{\mathbf{v}} \cdot \nabla \xi \quad \text{a.e. in } Q \end{aligned}$$

$$\bar{w}(x, t) = \int_{\Omega} k(|x-y|)(1 - 2\bar{\varphi}(y, t)) dy \quad \text{a.e. in } Q$$

$$\left(c_0 \nabla \xi + m'(\bar{\varphi}) \xi \nabla \bar{w} - 2 m(\bar{\varphi}) \nabla \left(\int_{\Omega} k(|x-y|) \xi(y, \cdot) dy \right) \right) \cdot \mathbf{n} = 0 \quad \text{a.e. on } \Sigma$$

$$\xi(0) = 0 \quad \text{a.e. in } \Omega$$

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Consider the linearized system obtained by linearizing the state system at $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$:

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We expect that the unique solution

$$\xi = DS(\bar{\mathbf{v}})\mathbf{h}$$

where $DS(\bar{\mathbf{v}})$ denotes the Fréchet derivative of \mathcal{S} at $\bar{\mathbf{v}}$.

Let the previous hypotheses be satisfied. Then the control-to-state operator

$$\mathcal{S} : \mathcal{V}_R \rightarrow C^1([0, T]; L^2(\Omega)) \cap H^1(0, T; H^1(\Omega)) \cap L^\infty(0, T; H^2(\Omega)), \quad \mathbf{v} \mapsto \varphi$$

is Fréchet differentiable in \mathcal{V}_R from \mathcal{V} into $\mathcal{Y} := C^0([0, T]; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$, and, for every $\bar{\mathbf{v}} \in \mathcal{V}_R$, $D\mathcal{S}(\bar{\mathbf{v}}) \in \mathcal{L}(\mathcal{V}, \mathcal{Y})$ is defined as follows: for every $\mathbf{h} \in \mathcal{V}$ we have

$$D\mathcal{S}(\bar{\mathbf{v}})\mathbf{h} = \xi^{\mathbf{h}}$$

where $\xi^{\mathbf{h}}$ is the unique solution to the linearized system with $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$.

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where $\xi^{\mathbf{h}}$ is the unique solution to the linearized system with $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$.

Assume that the previous hypotheses are fulfilled, and let $\bar{\mathbf{v}} \in \mathcal{V}_{\text{ad}}$ be an optimal control for problem **(CP)** with associated state $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$. Then we have for every $\mathbf{v} \in \mathcal{V}_{\text{ad}}$ the inequality

$$\begin{aligned} & \beta_1 \int_0^T \int_{\Omega} (\bar{\varphi} - \varphi_Q) \xi^{\mathbf{h}} \, dx \, ds + \beta_2 \int_{\Omega} (\bar{\varphi}(T) - \varphi_{\Omega}) \xi^{\mathbf{h}}(T) \, dx \quad \text{(VAR)} \\ & + \beta_3 \int_0^T \int_{\Omega} \bar{\mathbf{v}} \cdot (\mathbf{v} - \bar{\mathbf{v}}) \, dx \, ds \geq 0 \end{aligned}$$

where $\xi^{\mathbf{h}}$ is the unique solution to the linearized system associated with $\mathbf{h} = \mathbf{v} - \bar{\mathbf{v}}$

In order to establish the necessary first-order optimality conditions for **(CP)**, we need to eliminate ξ^h from inequality **(VAR)**. To this end, we introduce the *adjoint system* which formally reads as follows:

$$-p_t - c_0 \Delta p - \nabla p \cdot \left[\bar{\mathbf{v}} + m'(\bar{\varphi}) \nabla \left(\int_{\Omega} k(|x-y|)(1-2\bar{\varphi}(y,t)) dy \right) \right]$$

$$- 2 \int_{\Omega} \nabla p(y,t) m(\bar{\varphi}(y,t)) \cdot \nabla k(|x-y|) dy = \beta_1(\bar{\varphi} - \varphi_Q) \quad \text{in } Q$$

$$\frac{\partial p}{\partial \mathbf{n}} = 0 \quad \text{on } \Sigma$$

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 \end{aligned}$$

The adjoint system has a unique solution

$$p \in H^1(0, T; H^1(\Omega)^*) \cap C^0([0, T]; L^2(\Omega)) \cap L^2(0, T; H^1(\Omega))$$

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Proof. We only note that we have

$$\begin{aligned} & \beta_1 \int_0^T \int_{\Omega} (\bar{\varphi} - \varphi_Q) \xi^{\mathbf{h}} \, dx \, dt + \beta_2 \int_{\Omega} (\bar{\varphi}(T) - \varphi_{\Omega}) \xi^{\mathbf{h}}(T) \, dx \\ &= \beta_1 \int_0^T \int_{\Omega} (\bar{\varphi} - \varphi_Q) \xi^{\mathbf{h}} \, dx \, dt + \int_0^T \left(\langle p_t(t), \xi^{\mathbf{h}}(t) \rangle + \langle \xi_t^{\mathbf{h}}(t), p(t) \rangle \right) \, dt \\ &= \int_0^T \int_{\Omega} p(\mathbf{v} - \bar{\mathbf{v}}) \cdot \nabla \bar{\varphi} \, dx \, dt \end{aligned}$$

where the last equality easily follows from expressing $p_t(t)$ and $\xi_t^{\mathbf{h}}(t)$ via the adjoint equation and the linearized system and then integrating by parts

Moreover, since \mathcal{V}_{ad} is a nonempty, closed, and convex subset of $L^2(Q)^3$, we can infer that for $\beta_3 > 0$ the optimal control $\bar{\mathbf{v}}$ is the $L^2(Q)^3$ -orthogonal projection of $-\beta_3^{-1} p \nabla \bar{\varphi}$ onto \mathcal{V}_{ad}

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$$\tilde{v}_i(x, t) := \max \left\{ \tilde{v}_{1_i}(x, t), \min \left\{ \tilde{v}_{2_i}(x, t), -\beta_3^{-1} p(x, t) \partial_i \bar{\varphi}(x, t) \right\} \right\}$$

for $i = 1, 2, 3$, and almost every $(x, t) \in Q$, belongs to \mathcal{V}_{ad} , then $\tilde{\mathbf{v}} = \bar{\mathbf{v}}$, and the optimal control $\bar{\mathbf{v}}$ turns out to be a pointwise projection

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However the requirement $\tilde{\mathbf{v}} \in \mathcal{V}_{\text{ad}}$ implies that we should have $\tilde{\mathbf{v}}_t \in L^2(0, T; L^3(\Omega)^3)$, which in general cannot be expected since we only can guarantee the regularity $p_t \in L^2(0, T; H^1(\Omega)^*)$

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Therefore, the information about the optimal control that can be recovered from the projection property may be rather weak, in general. This is in contrast to the non-convective local case (see, e.g., [Hintermüller, Wegner, '12]) and to the convective local 2D case (see [Zhao, Liu, '14], where different boundary conditions are considered); it is in fact the price to be paid for considering the three-dimensional case with the flow velocity as the control parameter.

Other interesting problems would be related to:

- the optimal control problem related to the coupling of **(P1)–(P4)** with a Navier–Stokes system governing the evolution of the velocity \mathbf{v} :

$$\mathbf{v}_t - 2 \operatorname{div} (\nu(\varphi) D\mathbf{v}) + (\mathbf{v} \cdot \nabla)\mathbf{v} + \nabla\pi = \mu \nabla\varphi + \mathbf{u}, \quad \operatorname{div}(\mathbf{v}) = 0$$

- The existence of weak solutions to such coupled systems and their long-time behavior have recently been studied in [Frigeri, Grasselli, Krejčí, '13] and [Frigeri, Grasselli, Rocca, '13] in the two- and three-dimensional cases
- The analysis of the associated **control problem in the 2D case** has been recently done in [Frigeri, E.R., Sprekels, '14] in case of regular potentials and constant mobilities (**cf. the next talk by Sergio Frigeri**)

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- **Open problems:** the case of more general potentials – possibly singular or of obstacle type – and mobilities – possibly degenerating