Weierstrass Institute for
Applied Analysis and Stochastics

Optimal control of a nonlocal convective Cahn-Hilliard equation by the velocity

Elisabetta Rocca – with Jürgen Sprekels (WIAS – Berlin) – preprint arXiv:1404.1765v2 (2014)

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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*

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

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

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

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

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

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

where $H^1_{div}(\Omega) := \{\mathbf{v} \in H^1_0(\Omega)^3 : \operatorname{div}(\mathbf{v}) = 0\}$

- The state system:
  - nonlocal vz 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 local case, cf. [Elliott, Garcke '96], [Boyer, '99], [Abels, '09], ...)

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

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

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

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

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

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

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

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Actually, we could consider the more general case when

$f \in C^4(0,1)$ is strictly convex in $(0,1)$, $Im(f')^{-1} = [0,1]$, $\dfrac{1}{f''}$ 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) $\int_\Omega \int_\Omega k(|x-y|)\, \mathrm{d}x\, \mathrm{d}y =: k_0 < +\infty, \quad \sup_{x\in\Omega} \int_\Omega |k(|x-y|)|\, \mathrm{d}y =: \bar{k} < +\infty$

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

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

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

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:

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

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- [Londen, Petzeltová, '11]: convergence to single equilibria and separation properties for the **nonlocal Cahn–Hilliard system** with degenerate mobility and singular potential

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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 $\Longrightarrow$ through the convective term there arises a nonlinear coupling between control and state in product form that renders the analysis difficult $\Longrightarrow$ 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 (inpurities) 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.

(H4) $\mathcal{V}_{\rm ad} := \{\mathbf{v} = (v_1, v_2, v_3) \in \mathcal{V} : \ \widetilde{v}_{1_i} \le v_i \le \widetilde{v}_{2_i}$ a.e. in $Q, \ i = 1, 2, 3,$

$$\|\mathbf{v}\|_{L^2(0,T;H^1_{div}(\Omega)^3)} + \|\mathbf{v}_t\|_{L^2(0,T;L^3(\Omega)^3)} \le V\Big\}$$

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

Observe that $\mathcal{V}_{\rm ad}$ 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:

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

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

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

$$0 = \left(c_0 \nabla\varphi_0 + m(\varphi_0) \nabla \int_\Omega k(|x-y|)(1 - 2\varphi_0(y))\,\mathrm{d}y\right) \cdot \mathbf{n}$$

$$= m(\varphi_0) \nabla\mu(\cdot, 0) \cdot \mathbf{n}.$$

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*

$$0 < \kappa \leq \varphi \leq 1 - \kappa < 1 \quad a.e.\ \ in\ \ Q\,.$$

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:

$$\int_0^t \|(\varphi_1 - \varphi_2)_t(s)\|^2_{L^2(\Omega)}\,\mathrm{d}s + \max_{0\leq s\leq t} \|(\varphi_1 - \varphi_2)(s)\|^2_{H^1(\Omega)} \leq$$

$$K_2^* \int_0^t \|(\mathbf{v}_1 - \mathbf{v}_2)(s)\|^2_{L^3(\Omega)^3}\,\mathrm{d}s$$

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

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

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 $\bar{\varphi} = S(\bar{\mathbf{v}})$:

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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 $\bar{\varphi} = S(\bar{\mathbf{v}})$:

$$\xi_t - c_0 \Delta\xi - \operatorname{div}\left(m'(\bar{\varphi})\,\xi\,\nabla\bar{w} - 2\,m(\bar{\varphi})\,\nabla\left(\int_\Omega k(|x-y|)\,\xi(y,\cdot)\,\mathrm{d}y\right)\right)$$

$$= -\,\mathbf{h}\cdot\nabla\bar{\varphi} - \bar{\mathbf{v}}\cdot\nabla\xi \quad \text{a.e. in } Q$$

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

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

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We expect that the unique solution

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

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

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

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

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 $\bar{\mathbf{v}} \in \mathcal{V}_{\mathrm{ad}}$ be an optimal control for problem **(CP)** with associated state $\bar{\varphi} = \mathcal{S}(\bar{\mathbf{v}})$. Then we have for every $\mathbf{v} \in \mathcal{V}_{\mathrm{ad}}$ the inequality

$$\beta_1 \int_0^T \int_\Omega (\bar{\varphi} - \varphi_Q)\, \xi^{\mathbf{h}} \, \mathrm{d}x \, \mathrm{d}s + \beta_2 \int_\Omega (\bar{\varphi}(T) - \varphi_\Omega)\, \xi^{\mathbf{h}}(T) \, \mathrm{d}x \qquad \textbf{(VAR)}$$

$$+ \beta_3 \int_0^T \int_\Omega \bar{\mathbf{v}} \cdot (\mathbf{v} - \bar{\mathbf{v}}) \, \mathrm{d}x \, \mathrm{d}s \geq 0$$

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 $\xi^{\mathbf{h}}$ from inequality (**VAR**). To this end, we introduce the *adjoint system* which formally reads as follows:

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

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

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

$$p(T) = \beta_2(\bar\varphi(T) - \varphi_\Omega) \quad \text{a.e. in } \Omega$$

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

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

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

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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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$$\beta_3 \int_0^T \int_\Omega \bar{\mathbf{v}} \cdot (\mathbf{v} - \bar{\mathbf{v}}) \, \mathrm{d}x \, \mathrm{d}t + \int_0^T \int_\Omega p(\mathbf{v} - \bar{\mathbf{v}}) \cdot \nabla \bar{\varphi} \, \mathrm{d}x \, \mathrm{d}t \geq 0$$

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Proof. We only note that we have

$$\beta_1 \int_0^T \int_\Omega (\bar{\varphi} - \varphi_Q) \, \xi^{\mathbf{h}} \, \mathrm{d}x \, \mathrm{d}t + \beta_2 \int_\Omega (\bar{\varphi}(T) - \varphi_\Omega) \, \xi^{\mathbf{h}}(T) \, \mathrm{d}x$$

$$= \beta_1 \int_0^T \int_\Omega (\bar{\varphi} - \varphi_Q) \, \xi^{\mathbf{h}} \, \mathrm{d}x \, \mathrm{d}t + \int_0^T \Big(\langle p_t(t), \xi^{\mathbf{h}}(t) \rangle + \langle \xi^{\mathbf{h}}_t(t), p(t) \rangle \Big) \, \mathrm{d}t$$

$$= \int_0^T \int_\Omega p \, (\mathbf{v} - \bar{\mathbf{v}}) \cdot \nabla \bar{\varphi} \, \mathrm{d}x \, \mathrm{d}t$$

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

Moreover, since $\mathcal{V}_{\mathrm{ad}}$ 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 $\mathcal{V}_{\mathrm{ad}}$

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

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

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However the requirement $\widetilde{\mathbf{v}} \in \mathcal{V}_{\rm ad}$ implies that we should have $\widetilde{\mathbf{v}}_t \in L^2(0,T;L^3(\Omega)^3)$, 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 case of more general potentials and mobilities and
- the optimal control problem related to the coupling of (**P1**)–(**P4**) with a Navier–Stokes system governing the evolution of the velocity $\mathbf{v}$:

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

  - 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