Weierstrass Institute for
Applied Analysis and Stochastics

A time discretization for a nonstandard viscous Cahn–Hilliard system

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(joint work with P. Colli, G. Gilardi, P. Podio-Guidugli and P. Krejčí)

Dedicated to Gianni!

We consider the modified Cahn–Hilliard system

$$(\varepsilon + 2g(\rho))\mu_t + \mu\, g'(\rho)\, \rho_t - \Delta\mu = 0 \quad \text{in} \quad Q := \Omega \times (0,T) \tag{1}$$

$$\rho_r - \Delta\rho + f'(\rho) = \mu\, g'(\rho) \quad \text{in} \quad Q \tag{2}$$

$$\partial_\nu\, \mu = \partial_\nu\, \rho = 0 \quad \text{on} \quad \Sigma := \partial\Omega \times (0,T) \tag{3}$$

$$\mu_{|t=0} = \mu^0, \quad \rho_{|t=0} = \rho^0 \quad \text{in} \quad \Omega \tag{4}$$

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- Model by P. Podio-Guidugli (2006) for phase segregation through atom rearrangement on a lattice
- Studied for the special case $g(\rho) = \rho$ in a series of papers by P. Colli, G. Gilardi, P. Podio-Guidugli and J. S. for the Allen–Cahn version (2010) and the Cahn–Hilliard version (2011 ff.) concerning well-posedness, optimal control and asymptotic behavior as $t \to \infty$ and $\varepsilon \searrow 0$.

General assumptions

- $\Omega \subset \mathbb{R}^M$ is an open and bounded domain with smooth boundary $\partial\Omega$ and outward unit normal field ν.

- $f = f_1 + f_2$, where $f_2 \in C^2[0,1]$, and where $f_1 \in C^2(0,1)$ is convex and satisfies $\lim_{r \searrow 0} f_1'(r) = -\infty$ and $\lim_{r \nearrow 1} f_1'(r) = +\infty$.

- $g \in W^{2,\infty}(0,1)$ and $g(\rho) \geq 0 \quad \forall\, \rho \in [0,1]$.

- $\mu^0 \in V \cap L^\infty(\Omega)$, and $\mu^0 \geq 0$ a.e. in Ω.

- $\rho^0 \in W$, $0 < \rho^0 < 1$ in $\overline{\Omega}$, and $f'(\rho^0) \in H$.

Here, we set: $V := H^1(\Omega)$, $H := L^2(\Omega)$, $W := \{v \in H^2(\Omega)\,;\, \partial_\nu v = 0 \text{ on } \partial\Omega\}$.

Well-posedness (see Gianni's talk)

In the recent CGPS paper

"Global existence and uniqueness for a singular/degenerate Cahn–Hilliard system with viscosity" (submitted, see WIAS preprint No. 1713 (2012))

it was shown that (1)–(4) has a unique solution (μ, ρ) having the following properties:

- $\mu \in H^1(0,T;H) \cap L^2(0,T;W) \cap L^\infty(Q)$
- $\rho \in W^{1,\infty}(0,T;H) \cap H^1(0,T;V) \cap L^\infty(0,T;W)$
- $\mu \geq 0$ a.e. in Q
- There exist ρ_* , $\rho^* \in (0,1)$ such that $\rho_* \leq \rho \leq \rho^*$ a.e. in Q .

A similar result can also be obtained under weaker conditions (see the above paper).

Aim of talk

In this talk, we make the first step towards the numerical approximation of (1)–(4). We choose $N \in \mathbb{N}$, put $h = \frac{T}{N}$, and consider for $0 \leq n \leq N-1$ the time-discretized problem (where we put $\varepsilon = 1$)

$$(1 + 2\, g(\rho_n))\, \frac{\mu_{n+1} - \mu_n}{h} + \frac{g(\rho_{n+1}) - g(\rho_n)}{h}\, \mu_{n+1} - \Delta \mu_{n+1} = 0 \quad \text{in } \Omega \qquad (5)$$

$$\frac{\rho_{n+1} - \rho_n}{h} - \Delta \rho_{n+1} + f'(\rho_{n+1}) = \mu_n\, g'(\rho_n) \quad \text{in } \Omega \qquad (6)$$

$$\partial_\nu\, \mu_{n+1} = \partial_\nu\, \rho_{n+1} = 0 \quad \text{on } \partial\Omega \qquad (7)$$

$$\mu_0 = \mu^0, \quad \rho_0 = \rho^0 \quad \text{in } \Omega \qquad (8)$$

AIM: Well-posedness of the scheme, convergence of discrete solutions to (μ, ρ) as $N \to \infty$, error estimates

Existence of the discrete solution I

We argue by induction for $n \in \mathbb{N}$. Suppose that for some $0 \le n < N-1$ we have found $(\mu_n, \rho_n) \in W \times W$ such that $\mu_n \ge 0$ a.e. in Ω, $f'(\rho_n) \in H$ and $0 < \rho_n < 1$ in $\overline{\Omega}$. We rewrite (5), (6) in the form

$$(1 + g(\rho_n) + g(\rho_{n+1}))\,\mu_{n+1} - h\,\Delta\mu_{n+1} = (1 + 2\,g(\rho_n))\,\mu_n \quad \text{in } \Omega \tag{9}$$

$$\rho_{n+1} - h\,\Delta\rho_{n+1} + h\,f'(\rho_{n+1}) = \rho_n + h\,\mu_n\,g'(\rho_n) \quad \text{in } \Omega \tag{10}$$

Now let $\tilde{f} = \tilde{f}_1 + \tilde{f}_2$, where

- $\tilde{f}_2$ is any smooth extension of f_2 to $\mathbb{R}$,
- $\tilde{f}_1$ is the unique convex and l.s.c. extension of f_1 to $\mathbb{R}$ that satisfies $\tilde{f}(r) = +\infty$ if $r \notin (0,1)$.

Then the function $r \longmapsto \frac{1}{2}r^2 + h\,\tilde{f}(r)$ is strictly convex provided that

$$h \max_{0 \le r \le 1} |f_2''(r)| < 1 \tag{11}$$

We will always assume this in the following.

Existence of the discrete solution II

For $h > 0$ satisfying (11), it follows from standard arguments that the strictly convex, coercive and l.s.c. functional $J : V \to (-\infty, +\infty]$,

$$J(v) = \begin{cases} \frac{h}{2}\int_\Omega |\nabla v|^2 dx + \int_\Omega \left(\frac{v^2}{2} + h\tilde{f}(v)\right) dx - \int_\Omega (\rho_n + h\mu_n g'(\rho_n))v\, dx, & \text{if } \tilde{f}(v) \in L^1(\Omega) \\ +\infty\,, & \text{otherwise} \end{cases}$$

has a unique minimizer ρ_{n+1} on V. Standard arguments (maximal monotonicity, Euler–Lagrange, elliptic regularity) then show that actually $\rho_{n+1} \in W$ solves (10) and that $0 < \rho_{n+1} < 1$ in $\overline{\Omega}$.

But then also $g(\rho_{n+1}) \geq 0$ in Ω, and the elliptic boundary value problem (9), $\partial_\nu \mu_{n+1} = 0$ on $\partial\Omega$, has a unique solution $\mu_{n+1} \in W$. Testing (9) by $-\mu_{n+1}^- \leq 0$ yields immediately that $\mu_{n+1} \geq 0$ a.e. in Ω.

Step 1: Test (5) by $h\,\mu_{n+1}$ $\Longrightarrow$

$$\frac{1}{2}\|\mu_{n+1}\|_H^2 + \frac{1}{2}\|\mu_{n+1}-\mu_n\|_H^2 - \frac{1}{2}\|\mu_n\|_H^2 + h\int_\Omega |\nabla\mu_{n+1}|^2\,dx$$

$$+\int_\Omega \left[g(\rho_{n+1})\mu_{n+1}^2 - g(\rho_n)\mu_n^2 + g(\rho_n)(\mu_{n+1}-\mu_n)^2\right]\,dx = 0$$

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Summation $\Longrightarrow$

$$\int_\Omega \left(\frac{1}{2}+g(\rho_n)\right)\mu_m^2\,dx + \sum_{n=0}^{m-1}\int_\Omega \left(\frac{1}{2}+g(\rho_n)\right)|\mu_{n+1}-\mu_n|^2\,dx$$

$$+h\sum_{n=0}^{m-1}\int_\Omega |\nabla\mu_{n+1}|^2\,dx \le C\,, \quad 1\le m\le N\,. \tag{12}$$

Step 2: Test (6) by $\rho_{n+1} - \rho_n \implies$

$$h \left\| \frac{\rho_{n+1} - \rho_n}{h} \right\|_H^2 + \frac{1}{2} \left(\left\| \nabla \rho_{n+1} \right\|_H^2 - \left\| \nabla \rho_n \right\|_H^2 + \left\| \nabla (\rho_{n+1} - \rho_n) \right\|_H^2 \right)$$

$$+ \int_\Omega \Big(f_1(\rho_{n+1}) - f_1(\rho_n) \Big)\, dx \le \int_\Omega C\, h \Big(1 + |\mu_n| \Big) \frac{\rho_{n+1} - \rho_n}{h}\, dx \,,$$

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using the boundedness of g' and f_2'. Young's inequality and summation over n yield

$$\sum_{n=0}^{m-1} h \left\| \frac{\rho_{n+1} - \rho_n}{h} \right\|_H^2 + \left\| \nabla \rho_m \right\|_H^2 + \sum_{n=0}^{m-1} \left\| \nabla(\rho_{n+1} - \rho_n) \right\|_H^2 + \int_\Omega f_1(\rho_m) \, dx \leq C. \tag{13}$$

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Step 3: Test (6) by $-h\,\Delta\rho_{n+1}$ and by $h\,f_1'(\rho_{n+1}) \implies$

$$\sum_{n=0}^{m-1} h\left\|\rho_n\right\|_W^2 + \sum_{n=0}^{m-1} h\left\|f_1'(\rho_m)\right\|_H^2 \le C \tag{14}$$

Step 4: Take the difference of (6), written for $n+1$ and n, and test by $h^{-1}(\rho_{n+2}-\rho_{n+1})$. We obtain

$$\frac{1}{2}\left[\left\|\frac{\rho_{n+2}-\rho_{n+1}}{h}\right\|_H^2 - \left\|\frac{\rho_{n+1}-\rho_n}{h}\right\|_H^2 + \left\|\frac{\rho_{n+2}-\rho_{n+1}}{h} - \frac{\rho_{n+1}-\rho_n}{h}\right\|_H^2\right]$$

$$+h\int_\Omega \left|\nabla \frac{\rho_{n+2}-\rho_{n+1}}{h}\right|^2 dx + \frac{1}{h}\int_\Omega \Big(f_1'(\rho_{n+2}) - f_1'(\rho_{n+1})\Big)(\rho_{n+2}-\rho_{n+1})\, dx$$

$$\leq \quad C\,h\left\|\frac{\rho_{n+2}-\rho_{n+1}}{h}\right\|_H^2 + C\,h\int_\Omega \mu_{n+1}\left|\frac{\rho_{n+2}-\rho_{n+1}}{h}\right|\left|\frac{\rho_{n+1}-\rho_n}{h}\right| dx$$

$$+\int_\Omega (\mu_{n+1}-\mu_n)\, g'(\rho_n)\, \frac{\rho_{n+2}-\rho_{n+1}}{h}\, dx\,.$$

One now substitutes for $\mu_{n+1}-\mu_n$ from (5). Young, Hölder, the embedding $V \hookrightarrow L^4(\Omega)$ and the discrete Gronwall lemma imply the estimate

A priori estimates IV

$$\left\|\frac{\rho_{m+1}-\rho_m}{h}\right\|_H^2+\sum_{n=0}^{m-1}\left\|\frac{\rho_{n+2}-\rho_{n+1}}{h}-\frac{\rho_{n+1}-\rho_n}{h}\right\|_H^2+\sum_{n=0}^{m-1}h\left\|\nabla\frac{\rho_{n+2}-\rho_{n+1}}{h}\right\|_H^2\le C. \tag{15}$$

Step 5: Write (5) in the form

$$\Big(1+g(\rho_n)+g(\rho_{n+1})\Big)\frac{\mu_{n+1}-\mu_n}{h}+\frac{g(\rho_{n+1})-g(\rho_n)}{h}\mu_n-\Delta\mu_{n+1}=0$$

and test by $h^{-1}(\mu_{n+1}-\mu_n)$. Hölder, Young, embeddings, discrete Gronwall $\Longrightarrow$

$$\sum_{n=0}^{m-1}h\left\|\frac{\mu_{n+1}-\mu_m}{h}\right\|_H^2+\left\|\nabla\mu_m\right\|_H^2+\sum_{n=0}^{m-1}\left\|\nabla(\mu_{n+1}-\mu_n)\right\|_H^2\le C\,. \tag{16}$$

From this, we can deduce further estimates by comparison.

Let $t_n = n\,h\,,\ 0 \le n \le N$. We define for $t_{n-1} < t \le t_n\,,\ 1 \le n \le N$:

$$\mu^h(t) = \mu_n\,, \quad \bar{\mu}^h = \mu_{n-1}\,, \quad \rho^h(t) = \rho_n\,, \quad \bar{\rho}^h(t) = \rho_{n-1}\,, \quad \xi^h(t) = f_1'(\rho_n)\,,$$

$$\tilde{\mu}^h(t) = \mu_{n-1} + \frac{1}{h}(t - t_{n-1})(\mu_n - \mu_{n-1})\,,\ \tilde{\rho}^h(t) = \rho_{n-1} + \frac{1}{h}(t - t_{n-1})(\rho_n - \rho_{n-1}),$$

$$\tilde{\eta}^h(t) = g(\rho_{n-1}) + \frac{1}{h}(t - t_{n-1})(g(\rho_n) - g(\rho_{n-1}))\,.$$

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Obviously, for $t_{n-1} < t \le t_n,\ 1 \le n \le N$, we have

$$\tilde{\mu}_t^h(t) = \frac{\mu_n - \mu_{n-1}}{h}\,, \quad \tilde{\rho}_t^h = \frac{\rho_n - \rho_{n-1}}{h}\,, \quad \tilde{\eta}_t^h = \frac{g(\rho_n) - g(\rho_{n-1})}{h}\,. \qquad (17)$$

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Notice that we have

$$\|\tilde{\mu}^h - \bar{\mu}^h\|_{L^2(Q)}^2 = \sum_{n=1}^{N} h^{-2}\|\mu_n - \mu_{n-1}\|_H^2 \int_{t_{n-1}}^{t_n} (t - t_{n-1})^2 dt = \frac{h}{3}\sum_{n=1}^{N} \|\mu_n - \mu_{n-1}\|_H^2 \le Ch. \tag{18}$$

Due to regularity of the time derivative of $\tilde{\mu}^h$, we even have

$$\|\tilde{\mu}^h - \bar{\mu}^h\|_{L^2(Q)}^2 = \frac{h^2}{3}\sum_{n=1}^{N} h \left\| \frac{\mu_n - \mu_{n-1}}{h} \right\|_H^2 = \frac{h^2}{3}\|\tilde{\mu}_t^h\|_{L^2(Q)}^2 \le C\,h^2. \tag{19}$$

Convergence I

Similar estimates can be proved for

$$\|\tilde{\mu}^h - \mu^h\|^2_{L^2(Q)}\,, \quad \|\mu^h - \bar{\mu}^h\|^2_{L^2(Q)}\,, \quad \|\tilde{\rho}^h - \rho^h\|^2_{L^2(Q)}\,, \quad \|\rho^h - \bar{\rho}^h\|^2_{L^2(Q)}.$$

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Owing to the a priori estimates, we have for $h \searrow 0$ (i.e., for $N \to \infty$):

$$\tilde{\mu}^h \to \mu \qquad \text{weakly star in } H^1(0,T;H) \cap L^\infty(0,T;V) \tag{20}$$

$$\mu^h \to \mu \qquad \text{weakly in } L^2(0,T;W) \tag{21}$$

$$\tilde{\mu}^h\,,\ \bar{\mu}^h\,,\ \mu^h \to \mu \qquad \text{strongly in } L^\infty(0,T;H) \quad \text{(by compactness)} \tag{22}$$

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$$\text{and strongly in } C^0([0,T];H) \tag{26}$$

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- Similarly, we find

$$\eta^h\,,\ \bar{\eta}^h \to g(\rho) \quad \text{strongly in } L^\infty(0,T;L^6(\Omega)) \quad \Longrightarrow$$
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- Similarly, we find

$$\eta^h\,,\ \bar\eta^h \to g(\rho) \quad \text{strongly in } L^\infty(0,T;L^6(\Omega)) \quad \Longrightarrow$$
$$\tilde\eta^h \to \eta \equiv g(\rho) \quad \text{strongly in } L^\infty(0,T;L^6(\Omega)) \qquad (28)$$

- Moreover,

$$\bar\mu^h\, g'(\bar\rho^h) \to \mu\, g'(\rho) \quad \text{strongly in } L^\infty(0,T;L^{3/2}(\Omega)) \qquad (29)$$
$$g(\bar\rho^h)\, \tilde\mu_t^h \to g(\rho)\, \mu_t \quad \text{weakly in } L^2(0,T;L^{3/2}(\Omega)) \qquad (30)$$
$$\tilde\eta_t^h\, \mu^h \to (g(\rho))_t\, \mu \quad \text{weakly in } L^2(0,T;L^{3/2}(\Omega)) \qquad (31)$$

Now observe that the discrete equations can be written as

$$(1 + 2\, g(\bar{\rho}^h))\, \tilde{\mu}_t^h \,+\, (\tilde{\eta}_t^h)\, \mu^h \,-\, \Delta\mu^h \,=\, 0 \quad \text{in } Q \tag{32}$$

$$\tilde{\rho}_t^h \,-\, \Delta\rho^h \,+\, \xi^h \,=\, \bar{\mu}^h\, g'(\bar{\rho}^h) \,-\, f_2'(\rho^h) \quad \text{in } Q \tag{33}$$

$$\partial_\nu\, \mu^h \,=\, \partial_\nu\, \rho^h \,=\, 0 \quad \text{on } \Sigma \tag{34}$$

$$\tilde{\mu}^h(0) \,=\, \mu^0\,, \quad \tilde{\rho}^h(0) \,=\, \rho^0\,, \quad \text{in } \Omega \tag{35}$$

It thus follows that the limit (μ, ρ) is the (unique) solution to (1)–(4) **!**

Error estimates

General strategy:

- Subtract (1) from (32) and test the difference by $(\tilde{\rho}^h - \rho)_t$.
- Subtract (2) from (33) and test the difference by $\tilde{\mu}^h - \mu$.
- Add the results.
- Estimate **!**

This strategy works in principle but requires lengthy estimates using similar techniques as in the derivation of the a priori estimates. However, one needs two preparatory results:

Preparation 1: We have for $0 < \varepsilon < 1$, by interpolation,

$$\|(\rho^h - \rho)(t)\|_{H^{2-\varepsilon}(\Omega)} \le C\,\|(\rho^h - \rho)(t)\|_V^{\alpha}\,\|(\rho^h - \rho)(t)\|_W^{1-\alpha}$$

for some $\alpha \in (0,1)$ depending on ε, and thus (23), (24) imply

$$\rho^h \to \rho \quad \text{strongly in } L^\infty(0,T;H^{2-\varepsilon}(\Omega)) \tag{36}$$

We infer that there are $\bar{N} \in \mathbb{N}$ and $\bar{r}, \hat{r}$ such that for any $N \ge \bar{N}$ it holds (where $h = h_N = \frac{T}{N}$)

$$0 < \bar{r} \le \rho\,,\ \rho^h\,,\ \bar{\rho}^h\,,\ \tilde{\rho}^h \le \hat{r} < 1 \tag{37}$$

Assuming $N \ge \bar{N}$ in the following, we can claim henceforth that f_1' and $f' = f_1' + f_2'$ are Lipschitz in the range of relevant arguments.

Preparation 2:

Under the further assumption $-\Delta\rho_0 + f'(\rho_0) - \mu_0\, g'(\rho_0) \in V$, which is satisfied if $\rho_0 \in H^3(\Omega)$, we can show that

$$\|\tilde{\rho}_t^h\|_{L^\infty(0,T;V)\cap L^2(0,T;W)} \leq C\,. \tag{38}$$

and

$$\|\Delta(\tilde{\rho}^h - \rho^h)\|_{L^2(0,T;H)} \leq C\,h^2\,. \tag{39}$$

We then obtain the following error estimate:

Theorem:

Let the general assumptions hold, and let $\rho_0 \in H^3$. Suppose that $N \in \mathbb{N}$ is so large that for $h = \frac{T}{N}$ we have:

- $\max_{0 \le r \le 1} |f_2''(r)| < \frac{1}{h}$.
- $0 < \bar{r} \le \rho, \rho^h, \bar{\rho}^h, \tilde{\rho}^h \le \hat{r} < 1$.

Then it holds

$$\|\tilde{\rho}^h - \rho\|_{H^1(0,T;H)\cap L^\infty(0,T;V)} + \|\tilde{\mu}^h - \mu\|_{L^\infty(0,T;H)\cap L^2(0,T;V)} \le C\, h^{1/2}, \qquad (40)$$

where $C > 0$ depends only on the data.

Remark: One obtains h in place of $h^{1/2}$ provided one can show that

$\|\nabla \tilde{\mu}_t^h\|_{L^2(Q)} \le C$. (Ongoing work; requires $\mu_0 \in W$)

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Ad multos annos, Gianni !