From nonlocal to local Cahn-Hilliard equation

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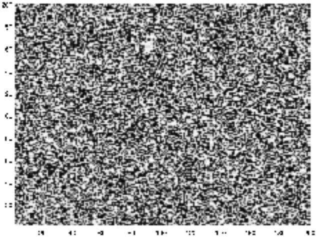
Cahn-Hilliard equation

- It has been proposed in 1958 by **[Cahn, Hilliard 1958, Cahn 1961]**
- It describes the process of phase separation (spinodal decomposition) in binary alloys (iron-nickel)
- Phase field model $u \in [0, 1]$ (vs sharp interface model $u \in \{0, 1\}$)
- It has a variety of applications:
  - image processing **[Capuzzo Dolcetta, Finzi Vita, March 2002]**
  - population dynamics **[Cohen, Murray 1981]**
  - formation of Saturn rings **[Tremaine 2003]**
  - tumour growth **[Colli, Garcke, Gilardi, Lam, Rocca, Sprekels, Scala . . .]**

Settings

$u \in \mathbb{R}$: real valued function representing the local concentration of one of the two components
$u = 0, u = 1$: pure phases



Two species A, B with concentrations c_A and $c_B = 1 - c_A$ at each point.
Then $u(x,t) = 1 - c_A(x,t)$ and:
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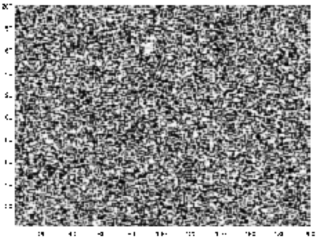

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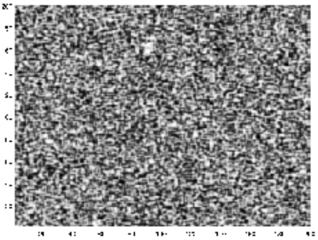

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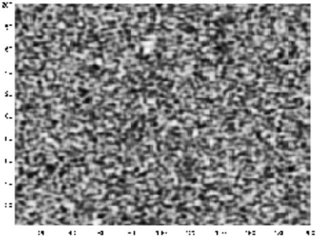

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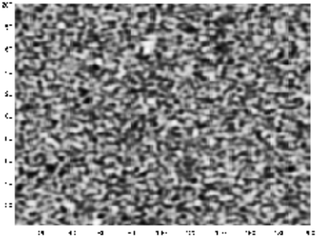

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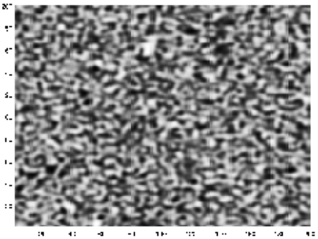

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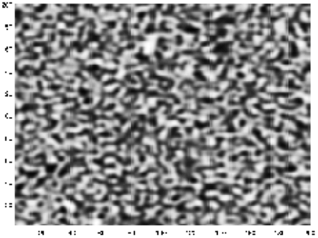

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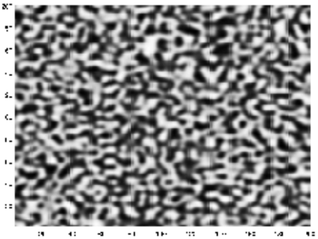

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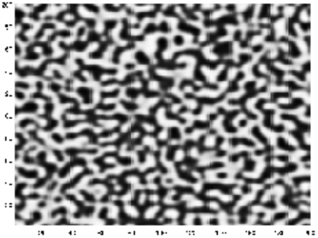

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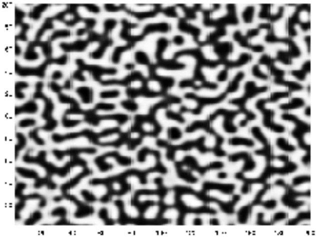

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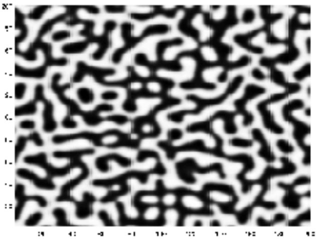

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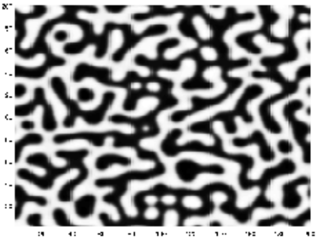

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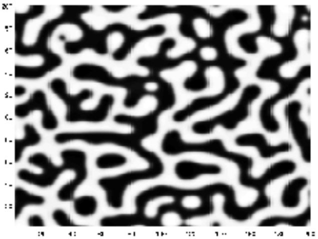

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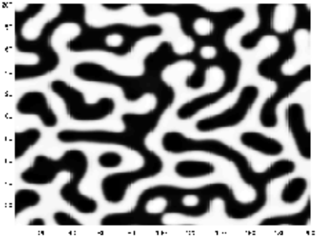

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Local Cahn-Hilliard

Free energy functional

$$E_{CH}(u) = \int_\Omega \Big(\frac{\tau^2}{2} |\nabla u|^2 + F(u) \Big) \, \mathrm{d}x$$

where

- τ: small positive parameter related to the transition region thickness
- F: double well potential with two global minima in the pure phases
- $|\nabla u|^2$: reflects intermolecular interactions (penalising the creation of interfaces)

Local Cahn-Hilliard

Corresponding evolution problem (4th order PDE):

$$\frac{\partial u}{\partial t} + \nabla \cdot J_{CH} = 0,$$
$$J_{CH} = -\mu(u)\nabla v_{CH},$$
$$v_{CH} = \frac{\delta E_{CH}(u)}{\delta u} = -\tau^2 \Delta u + F'(u)$$

where

- μ: mobility (constant $= 1$)
- $v = \frac{\delta E}{\delta u}$: chemical potential

Nonlocal Cahn-Hilliard

Proposed by **[Giacomin, Lebowitz 1997]**

Free energy functional

$$E_{NL}(u) = \frac{1}{4}\int_\Omega \int_\Omega K(x,y)(u(x)-u(y))^2 \mathrm{d}x\mathrm{d}y + \int_\Omega F(u(x))\mathrm{d}x,$$

where

- $K(x,y)$: positive and symmetric convolution kernel
- F: double well potential with two global minima in the pure phases

Nonlocal Cahn-Hilliard

Corresponding evolution problem (2^{nd} order PDE):

$$\begin{aligned}\frac{\partial u}{\partial t} + \nabla \cdot J_{NL} &= 0,\\ J_{NL} &= -\mu(u)\nabla v_{NL},\\ v_{NL} &= \frac{\delta E_{NL}(u)}{\delta u} = (K * 1)u - K * u + F'(u)\end{aligned}$$

Nonlocal Cahn-Hilliard

Corresponding evolution problem (2^{nd} order PDE):

$$\frac{\partial u}{\partial t} + \nabla \cdot J_{NL} = 0,$$

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$$v_{NL} = \frac{\delta E_{NL}(u)}{\delta u} = (K * 1)u - K * u + F'(u)$$

Goal: prove the convergence of solutions of the nonlocal Cahn-Hilliard equation to solutions of the local version in a periodic setting.

Local vs nonlocal

- They share fundamental features: underlying gradient flow structure, lack of comparison principle, separation from the pure phases,. . .
- Both energy functionals allow the same Γ-limit for vanishing interface thickness **[Gal, Grasselli, Miranville, Rocca,. . .]**
- Pointwise convergence is of little use due to non convexity and lack of coercivity of the nonlocal energy functional E_{NL} in H^1.
- There exists Γ-convergence for the energy functionals **[Ponce 2004]** but it is not trivial to prove convergence for solutions of the corresponding dynamic problems using **[Sandier, Serfaty 2011]**

Overview of known results and properties

Eq	F	μ	Existence	Separation	Long time
CH	pol	non-deg	Garcke '00, Temam	probably false	Temam '88
		deg	Elliott Garcke '96	?	?
	log	non-deg	Elliott Luckhaus '91	Miranville Zelik '04	Cherfils Zelik Miranville '11
		deg	Elliott Garcke '96	?	Debussche Dettori '95
NLCH	pol	non-deg	Bates Han '04	probably false	Gal Grasselli '17
		deg	?	?	?
	log	non-deg	Gal Giorgini Grasselli '17	Gal Giorgini Grasselli '17	Gal Giorgini Grasselli '17
		deg	Gajewski Zacharias '03	Londen Petzeltova '11	Londen Petzeltova '11

Hypothesis

H1 Ω d-dimensional flat torus with $d \leq 3$

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H2 Family of convolution kernels parametrised by a parameter ε:

$$K_\varepsilon(x, y) = \varepsilon^{-d-2} J\left(\left|\frac{x-y}{\varepsilon}\right|^2\right)$$

with $J : \mathbb{R} \to \mathbb{R}$ sufficiently smooth nonnegative function with compact support and

$$\frac{1}{d} \int_\Omega J(|z|^2)|z|^2 \, \mathrm{d}z = 1$$

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$$\frac{1}{d}\int_\Omega J(|z|^2)|z|^2 \,\mathrm{d}z = 1$$
- H3 $F \in C^2(\mathbb{R})$ double well potential with two global minima at 0 and 1 such that $F''(s) \geq 0$ for $s \in (-\infty, -a] \cup [a, +\infty)$ with a nonnegative, and $C_l(|u|^3 + 1) \leq F'(u) \leq C_u(|u|^3 + 1)$ for $C_l, C_u > 0$

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- H4 $u_{0,\varepsilon} \in L^2(\Omega)$ converges strongly in $L^2(\Omega)$ to the limit $u_0 \in H^1(\Omega)$ and satisfies $E_\varepsilon(u_{0,\varepsilon}), E(u_0) \leq C_0$ for some constant $C_0 > 0$ independent of ε

Definition of solutions

Definition (Weak solution to the nonlocal Cahn-Hilliard equation)

Let $\varepsilon > 0$ and $T > 0$ be fixed. We define u_ε to be a *weak solution* to the **nonlocal** Cahn-Hilliard equation on $[0, T]$ associated with the initial datum $u_{0,\varepsilon} \in L^2(\Omega)$ if

$$u_\varepsilon \in H^1(0,T;(H^1(\Omega))^*) \cap L^2(0,T;H^1(\Omega)),$$

satisfies

$$\langle \partial_t u_\varepsilon, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} + \int_\Omega \nabla[(K_\varepsilon * 1)u_\varepsilon - K_\varepsilon * u_\varepsilon + F'(u_\varepsilon)] \cdot \nabla\varphi \, \mathrm{d}x = 0$$

for all $\varphi \in H^1(\Omega)$, and $u_\varepsilon(0) = u_{0,\varepsilon}$.

Definition of solutions

Definition (Weak solution to the local Cahn-Hilliard equation)

Let $T > 0$ be fixed. We define u to be a *weak solution* to the Cahn-Hilliard equation on $[0, T]$ associated with the initial datum $u_0 \in H^1(\Omega)$ if

$$u \in H^1(0, T; (H^1(\Omega))^*) \cap L^2(0, T; H^2(\Omega)),$$

satisfies

$$\langle \partial_t u, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} + \int_\Omega \Delta u \Delta \varphi \, \mathrm{d}x - \int_\Omega F'(u) \Delta \varphi \, \mathrm{d}x = 0$$

for all $\varphi \in H^2(\Omega)$, and $u(0) = u_0$.

Main result

Remark:

- existence and uniqueness of weak solutions to both problems are well known with different choices for the boundary conditions
- both systems have been largely studied (qualitative properties, numerical aspects, long-time behaviour, asymptotics with different kinds of boundary conditions and different potentials)

Main result

Remark:

- existence and uniqueness of weak solutions to both problems are well known with different choices for the boundary conditions
- both systems have been largely studied (qualitative properties, numerical aspects, long-time behaviour, asymptotics with different kinds of boundary conditions and different potentials)

Theorem

Let u_ε be a solution of the nonlocal CH with periodic boundary conditions and kernel $K_\varepsilon(x,y)$.
Then $u_\varepsilon \to u$ in $L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^{-1}(\Omega))$ where u is a solution of the local CH.

Some comments

- Note that in the Neumann case CH has two boundary conditions (one for u and one for the chemical potential), while NLCH has just one (for the chemical potential v).
- The mobility can be annoying for the estimates on the chemical potential.

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- The mobility can be annoying for the estimates on the chemical potential.

Idea: use advantage of the dynamic structure:
for every fixed ε, $u_\varepsilon \in H^1$

Proof: uniform estimates

$$\langle \partial_t u_\varepsilon, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} + \int_\Omega \nabla[(K_\varepsilon * 1)u_\varepsilon - K_\varepsilon * u_\varepsilon + F'(u_\varepsilon)] \cdot \nabla\varphi \, \mathrm{d}x = 0$$

Test function: $\varphi = u_\varepsilon$

$$0 = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_\varepsilon\|^2_{L^2(\Omega)} + \int_\Omega \nabla \left[(K_\varepsilon * 1)u_\varepsilon - K_\varepsilon * u_\varepsilon + F'(u_\varepsilon)\right] \cdot \nabla u_\varepsilon \, \mathrm{d}x$$

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$$0 = \frac{1}{2} \frac{\mathrm{d}}{\mathrm{d}t} \|u_\varepsilon\|^2_{L^2(\Omega)} + \int_\Omega [\underbrace{(K_\varepsilon * 1)|\nabla u_\varepsilon|^2 - (K_\varepsilon * \nabla u_\varepsilon) \cdot \nabla u_\varepsilon}_{\frac{1}{2} \int_\Omega \int_\Omega K_\varepsilon(x,y) |\nabla u_\varepsilon(x) - \nabla u_\varepsilon(y)|^2 \, \mathrm{d}x \, \mathrm{d}y} + F''(u_\varepsilon)|\nabla u_\varepsilon|^2] \, \mathrm{d}x$$

Proof: uniform estimates

Change of variable $\frac{x-y}{\varepsilon} =: z$

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_\varepsilon\|^2_{L^2(\Omega)} + \frac{1}{2}\int_\Omega\int_\Omega J(|z|^2)\left|\frac{\nabla u_\varepsilon(y+\varepsilon z) - \nabla u_\varepsilon(y)}{\varepsilon}\right|^2 \mathrm{d}y\,\mathrm{d}z$$

$$= -\int_\Omega F''(u_\varepsilon)|\nabla u_\varepsilon|^2\,\mathrm{d}x \leq B_1\|\nabla u_\varepsilon\|^2_{L^2(\Omega)}.$$

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Aim: estimate the blue term with $\|\nabla u_\varepsilon\|^2$

Key idea: **[Ponce 2004]**, Poincaré type inequality

Key idea

$\Omega \in \mathbb{R}^N$ with $N \geq 1$, bounded domain with Lipschitz boundary, $1 \leq p < \infty$

Poincaré

It exist $C_p > 0$ s.t.

$$\int_\Omega |f - f_\Omega|^p \leq C_p \int_\Omega |Df|^p, \quad \forall f \in W^{1,p}(\Omega)$$

Let $(\rho_n) \subset L^1(\mathbb{R}^N)$ be a sequence of radial functions satisfying:

$$\rho_n \geq 0 \qquad \text{a.e. in } \mathbb{R}^N$$

$$\int_{\mathbb{R}^N} \rho_n = 1 \qquad \forall n \geq 1$$

$$\lim_{n\to\infty} \int_{|h|>\delta} \rho_n(h)dh = 0 \qquad \forall \delta > 0$$

Theorem 1

Let $(\rho_n) \subset L^1(\mathbb{R}^N)$ be a sequence of radial functions as defined before. Given $\delta > 0$, there exists $n_0 \geq 1$ sufficiently large, such that

$$\int_\Omega |f - f_\Omega|^p \leq \left(\frac{C_p}{K_{p,N}} + \delta \right) \int_\Omega \int_\Omega \frac{|f(x) - f(y)|^p}{|x - y|^p} \rho_n(|x - y|) \, \mathrm{d}x \, \mathrm{d}y$$

for every $f \in L^p(\Omega)$ and $n \geq n_0$.

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Observe: this formulation is stronger than Poincaré.
It is easy to see that

$$\int_\Omega \int_\Omega \frac{|f(x) - f(y)|^p}{|x - y|^p} \rho_n(|x - y|) \, \mathrm{d}x \, \mathrm{d}y \leq \int_{\mathbb{R}^N} |Df|^p \leq C \int_\Omega |Df|^p$$

Theorem 2 – compactness

If $(f_n) \subset L^p(\mathbb{R}^n)$ is a bounded sequence such that

$$\int_\Omega \int_\Omega \frac{|f_n(x) - f_n(y)|^p}{|x-y|^p} \rho_n(|x-y|) dxdy \leq B, \quad \forall n \geq 1$$

then (f_n) is relatively compact in L^p.

Assume that $f_n \to f$ in $L^p(\Omega)$ then

- $f \in W^{1,p}(\Omega)$ if $1 < p < \infty$
- $f \in BV(\Omega)$ if $p = 1$

Proof: uniform estimates

$$\langle \partial_t u_\varepsilon, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} + \int_\Omega \nabla[(K_\varepsilon * 1)u_\varepsilon - K_\varepsilon * u_\varepsilon + F'(u_\varepsilon)] \cdot \nabla\varphi \, \mathrm{d}x = 0$$

Test function: $\varphi = (-\Delta)^{-1} U_\varepsilon$
where

$$(-\Delta)^{-1} : (H^1(\Omega))^* \to H^1(\Omega)$$

is the map assigning to every $v \in (H^1(\Omega))^*$ the unique solution w of the equation $-\Delta w = v$ such that the mean value is zero, i.e. $\overline{w} = 0$. We define $U_\varepsilon = u_\varepsilon - \overline{u_\varepsilon}$.

Proof: uniform estimates

$$\langle \partial_t u_\varepsilon, \varphi \rangle_{(H^1(\Omega))^*, H^1(\Omega)} + \int_\Omega \nabla[(K_\varepsilon * 1)u_\varepsilon - K_\varepsilon * u_\varepsilon + F'(u_\varepsilon)] \cdot \nabla\varphi \, \mathrm{d}x = 0$$

Test function: $\varphi = (-\Delta)^{-1} U_\varepsilon$
where

$$(-\Delta)^{-1} : (H^1(\Omega))^* \to H^1(\Omega)$$

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$$\|u_\varepsilon - \overline{u_\varepsilon}\|^2_{L^2(\Omega)} \leq C_p \int_\Omega \int_\Omega J(|z|^2)|z|^2 \left(\frac{U_\varepsilon(y + \varepsilon z) - U_\varepsilon(y)}{\varepsilon |z|} \right)^2 \mathrm{d}y \, \mathrm{d}z \leq B_2 |\Omega|$$

and

$$\|\nabla u_\varepsilon - \overline{\nabla u_\varepsilon}\|^2_{L^2(\Omega)} \leq C_p \int_\Omega \int_\Omega J(|z|^2)|z|^2 \left| \frac{\nabla u_\varepsilon(y + \varepsilon z) - \nabla u_\varepsilon(y)}{\varepsilon |z|} \right|^2 \mathrm{d}y \, \mathrm{d}z,$$

Uniform estimates

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_\varepsilon\|^2_{L^2(\Omega)} + \frac{1}{2}\int_\Omega\int_\Omega J(|z|^2)\left|\frac{\nabla u_\varepsilon(y+\varepsilon z) - \nabla u_\varepsilon(y)}{\varepsilon}\right|^2 \mathrm{d}y\,\mathrm{d}z \leq B_1\|\nabla u_\varepsilon\|^2_{L^2(\Omega)}$$

Uniform estimates

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_\varepsilon\|^2_{L^2(\Omega)} + \frac{1}{2}\int_\Omega\int_\Omega J(|z|^2)\left|\frac{\nabla u_\varepsilon(y+\varepsilon z) - \nabla u_\varepsilon(y)}{\varepsilon}\right|^2 \mathrm{d}y\,\mathrm{d}z \le B_1\|\nabla u_\varepsilon\|^2_{L^2(\Omega)}$$

$$\frac{1}{2}\|u_\varepsilon(T)\|^2_{L^2(\Omega)} + \left(\frac{1}{2C_p} - B_1\right)\|\nabla u_\varepsilon\|^2_{L^2(0,T;L^2(\Omega))} \le \frac{1}{2}\|u_\varepsilon(0)\|^2_{L^2(\Omega)}$$

Uniform estimates

$$\frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\|u_\varepsilon\|^2_{L^2(\Omega)} + \frac{1}{2}\int_\Omega\int_\Omega J(|z|^2)\left|\frac{\nabla u_\varepsilon(y+\varepsilon z)-\nabla u_\varepsilon(y)}{\varepsilon}\right|^2 \mathrm{d}y\,\mathrm{d}z \leq B_1\|\nabla u_\varepsilon\|^2_{L^2(\Omega)}$$

$$\frac{1}{2}\|u_\varepsilon(T)\|^2_{L^2(\Omega)} + \left(\frac{1}{2C_p} - B_1\right)\|\nabla u_\varepsilon\|^2_{L^2(0,T;L^2(\Omega))} \leq \frac{1}{2}\|u_\varepsilon(0)\|^2_{L^2(\Omega)}$$

$$\int_0^T\int_\Omega\int_\Omega J(|z|^2)\left|\frac{\nabla u_\varepsilon(y+\varepsilon z)-\nabla u_\varepsilon(y)}{\varepsilon}\right|^2 \mathrm{d}y\,\mathrm{d}z\,\mathrm{d}t \leq C$$

Proof: convergence

Goal: prove the limit u to be a weak solution of the local Cahn-Hilliard equation

$$
\begin{aligned}
u_\varepsilon &\rightharpoonup u && \text{weakly in } L^2(0,T;H^1(\Omega)) \\
\partial_t u_\varepsilon &\rightharpoonup \partial_t u && \text{weakly in } L^2(0,T;(H^1(\Omega))^*) \\
u_\varepsilon &\to u && \text{strongly in } C([0,T];L^2(\Omega))
\end{aligned}
$$

for some limit $u \in L^2(0,T;H^1(\Omega)) \cap H^1(0,T;(H^1(\Omega))^*)$

Proof: convergence

Goal: prove the limit u to be a weak solution of the local Cahn-Hilliard equation

$$\begin{aligned} u_\varepsilon &\rightharpoonup u && \text{weakly in } L^2(0,T;H^1(\Omega)) \\ \partial_t u_\varepsilon &\rightarrow \partial_t u && \text{weakly in } L^2(0,T;(H^1(\Omega))^*) \\ u_\varepsilon &\rightarrow u && \text{strongly in } C([0,T];L^2(\Omega)) \end{aligned}$$

for some limit $u \in L^2(0,T;H^1(\Omega)) \cap H^1(0,T;(H^1(\Omega))^*)$

[Ponce 2004] $\Rightarrow$ $u \in L^2(0,T;H^2(\Omega))$

Proof: convergence

Test function: $\varphi \in C^\infty(\Omega)$

$$0 = \underbrace{\int_0^T \int_\Omega (\partial_t u_\varepsilon)\varphi \,\mathrm{d}x\,\mathrm{d}t}_{I} - \underbrace{\int_0^T \int_\Omega F'(u_\varepsilon)\Delta\varphi \,\mathrm{d}x\,\mathrm{d}t}_{II}$$

$$\underbrace{-\frac{1}{2}\int_0^T \int_\Omega \int_\Omega K_\varepsilon(x,y)(u_\varepsilon(x) - u_\varepsilon(y))(\Delta\varphi(x) - \Delta\varphi(y))\,\mathrm{d}y\,\mathrm{d}x\,\mathrm{d}t}_{III}$$

(I)–(II): the growth conditions and continuity on F' suffice to pass to the limit

Proof: convergence

Thanks to (H2):

$$\frac{1}{d}\mathcal{H}^{d-1}(\mathcal{S}^{d-1})\int_0^\infty J(r^2)r^{d+1}\,\mathrm{d}r = 1$$

and by using the weak convergence:

$$\frac{1}{2}\int_0^T\int_\Omega J(|z|^2)|z|^2$$
$$\int_\Omega \frac{(u_\varepsilon(y+\varepsilon z)-u_\varepsilon(y))}{\varepsilon|z|}\frac{(\Delta\varphi(y+\varepsilon z)-\Delta\varphi(y))}{\varepsilon|z|}\mathrm{d}y\,\mathrm{d}z\mathrm{d}t$$
$$\to \frac{1}{2}\int_0^T\int_\Omega \nabla u(y)\cdot\nabla\Delta\varphi(y)\mathrm{d}y\,\mathrm{d}t$$

Thus, the limit u satisfies

$$\int_0^T\int_\Omega(\partial_t u)\varphi\,\mathrm{d}x\,\mathrm{d}t - \int_0^T\int_\Omega \nabla u\cdot\nabla\Delta\varphi\,\mathrm{d}x\,\mathrm{d}t - \int_0^T\int_\Omega F'(u)\Delta\varphi\,\mathrm{d}x\,\mathrm{d}t = 0.$$

Outlook and open questions

- Proved the convergence of weak solutions of the NLCH equation to the weak solutions to the local one as the convolution kernel approximates a Dirac delta (case with periodic boundary conditions) using a compactness argument.
- Dirichlet / Neumann boundary conditions?

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Thanks for your attention

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