Cahn-Hilliard and Thin film equations with nonlinear mobility as gradient flows in weighted Wasserstein metrics

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Outline

1 Evolution PDE's with a gradient flow structure

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2. The dynamical approach to weighted transport distances

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A general class of evolutionary PDE's

In many applications one is interested in **nonnegative integrable solutions** to evolution equations of the type

$$\partial_t u - \operatorname{div}\left(\mathfrak{m}(\mathbf{u})\mathrm{D}\frac{\delta\Phi}{\delta\mathbf{u}}\right) = 0 \quad \text{in } \Omega\times(0,\infty), \quad \Omega\subset\mathbb{R}^d,$$

with Neumann-variational boundary conditions

$$\mathbf{n}\cdot\mathrm{D}u = 0, \qquad \mathbf{n}\cdot\mathrm{D}\left(\mathfrak{m}(\mathbf{u})\frac{\delta\Phi}{\delta u}\right) = 0$$

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Drift-diffusion-interaction ($\mathfrak{m}(\mathbf{u}) = \mathbf{u}$):

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Chemotaxis with overcrowding prevention [Hillen-Painter '01]:

$$\partial_t u = \operatorname{div}\Big(\mathrm{D}u + \mathfrak{m}(\mathbf{u})\mathrm{D}(W * u)\Big) = \operatorname{div}\Big(\mathfrak{m}(\mathbf{u})\mathrm{D}\big(\mathbf{F}'(\mathbf{u}) + \mathbf{W} * \mathbf{u}\big)\Big)$$

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DLSS - Quantum drift-diffusion

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[Elliott-Garcke '96]

The gradient flow structure: a formal motivation

$$\partial_t u + \operatorname{div} \mathbf{w} = 0, \qquad \psi = \frac{\boldsymbol{\delta\Phi}}{\boldsymbol{\delta u}}$$

$$\frac{\mathrm{d}}{\mathrm{d}t}\boldsymbol{\Phi}(\mathbf{u_t}) = \int_{\mathbb{R}^d} \partial_t u \frac{\boldsymbol{\delta\Phi}}{\boldsymbol{\delta u}}\,\mathrm{d}x = -\int_{\mathbb{R}^d} (\operatorname{div} \mathbf{w})\psi\,\mathrm{d}x = \int_{\mathbb{R}^d} \mathbf{w}\cdot \mathbf{D}\psi\,\mathrm{d}x$$

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$$\partial_t u + \operatorname{div} \mathbf{w} = 0, \quad \mathbf{w} = \mathfrak{m}(\mathbf{u})\mathbf{v} \qquad\qquad \psi = \frac{\delta \Phi}{\delta \mathbf{u}}$$

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$$\Big(\int_{\mathbb{R}^d} |\mathbf{v}|^2 \mathfrak{m}(\mathbf{u}) \,\mathrm{d}x\Big)^{1/2}$$

as the "velocity" of the moving family u.

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If we want to decrease $\mathbf{\Phi}$ as fast as possible, we have to choose

$$\boxed{\mathbf{v} = -\mathbf{D}\psi}$$

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3 Basic tools for metric gradient flows: displacement convexity, variational approximation (JKO and WED schemes), flow interchange.

Weighted transport distances: the dynamical approach

[Benamou-Brenier '00]
We interpret u as the density of a (probability) measure $\rho = u\,\mathrm{d}x$ and we consider a time dependent family $\mathbf{u}_t$, $t \in [0, T]$, of densities satisfying the **nonlinear continuity equation**

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The **scalar velocity** at time t is given by

$$\mathcal{V}_\mathbf{t}[\mathbf{u}_t] := \|\mathbf{v}_\mathbf{t}\|_{L^2(\mathfrak{m}(u_t);\mathbb{R}^d)} = \left(\int_{\mathbb{R}^d} |\mathbf{v}_\mathbf{t}(\mathbf{x})|^2\,\mathfrak{m}(\mathbf{u}_\mathbf{t})\,\mathrm{d}x\right)^{1/2}.$$

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The length of the curve $\mathbf{u}$ between t_0 and t_1

$$\mathcal{L}_{t_0}^{t_1}[\mathbf{u}] := \int_{t_0}^{t_1} \mathcal{V}_t[\mathbf{u}]\,\mathrm{d}t = \int_{t_0}^{t_1}\left(\int_{\mathbb{R}^d} |\mathbf{v_t(x)}|^2\,\mathfrak{m}(\mathbf{u_t})\,\mathrm{d}x\right)^{1/2}\mathrm{d}t$$

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[Benamou-Brenier '00]
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$$\boxed{\partial_t \mathbf{u} + \operatorname{div}\big(\mathfrak{m}(\mathbf{u})\,\mathbf{v}\big) = 0}$$

The **scalar velocity** at time t is given by

$$\mathcal{V}_{\mathbf{t}}[\mathbf{u}_t] := \|\mathbf{v}_{\mathbf{t}}\|_{L^2(\mathfrak{m}(u_t);\mathbb{R}^d)} = \Big(\int_{\mathbb{R}^d} |\mathbf{v}_{\mathbf{t}}(\mathbf{x})|^2\,\mathfrak{m}(\mathbf{u}_{\mathbf{t}})\,\mathrm{d}x\Big)^{1/2}.$$

The length of the curve $\mathbf{u}$ between t_0 and t_1

$$\mathcal{L}_{t_0}^{t_1}[\mathbf{u}] := \int_{t_0}^{t_1} \mathcal{V}_t[\mathbf{u}]\,\mathrm{d}t = \int_{t_0}^{t_1} \Big(\int_{\mathbb{R}^d} |\mathbf{v}_{\mathbf{t}}(\mathbf{x})|^2\,\mathfrak{m}(\mathbf{u}_{\mathbf{t}})\,\mathrm{d}x\Big)^{1/2}\mathrm{d}t$$

Weighted transport distance $\mathrm{W}_{\mathfrak{m}}$ between $\mathbf{u}_0$ and $\mathbf{u}_1$:

$$\mathrm{W}_{\mathfrak{m}}(\mathbf{u}_0, \mathbf{u}_1) := \min\Big\{\mathcal{L}_0^1[\mathbf{u}] : \mathbf{u}\big|_{t=0} = \mathbf{u}_0,\ \mathbf{u}\big|_{t=1} = \mathbf{u}_1\Big\}.$$

Limiting cases

$\mathfrak{m}(\mathbf{r}) \equiv \mathbf{1}$ $\leftrightarrow$ **Homogeneous dual $W^{-1,2}(\mathbb{R}^d)$ distance.**

$$\mathrm{W}_{\mathfrak{m}}(\mathbf{u}_0, \mathbf{u}_1) = \sup \left\{ \int_{\mathbb{R}^d} (\mathbf{u}_0 - \mathbf{u}_1)\varphi \,\mathrm{d}x : \int_{\mathbb{R}^d} |\mathrm{D}\varphi|^2 \,\mathrm{d}x \le 1 \right\}$$

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[Jordan-Kinderlehrer-Otto '98, Otto '01]
Applications: optimal transport, existence and asymptotic behaviour of solutions, contraction properties, Logarithmic Sobolev Inequalities, approximation algorithms, curvature and metric measure spaces, stability,...
[Ambrosio-Gigli-S., Agueh, Brenier, Carrillo, Carlen, McCann, Gangbo, Giacomelli, Gianazza-Toscani-S., Lisini, Otto, Slepcev, Sturm, Villani, Westdickenberg, ...]

The interest of the method and the main problems

ADVANTAGES

- **Non-negativity** is for free.
- A general **approximation scheme**, which is a variational formulation of the backward Euler method, is always available.
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- Are there interesting **convexity properties** of the integral functionals and related **functional inequalities** ?

The variational problem

Problem

Given nonnegative densities $u_0, u_1 \in L^1_{\mathrm{loc}}(\mathbb{R}^d)$ *find a minimizer of the action functional*

$$\int_0^1 \int_{\mathbb{R}^d} |\mathbf{v_t}|^2 \mathfrak{m}(\mathbf{u_t}) \,\mathrm{d}x \,\mathrm{d}t \quad s.t. \quad \partial_t u + \mathrm{div}(\mathfrak{m}(\mathbf{u_t})\mathbf{v_t}) = 0, \quad u_{|_{t=0,1}} = u_{0,1}.$$

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Direct method of the calculus of variations: fix the densities u_0, u_1 and take a minimizing sequence $(u_t^n, \mathbf{w}_t^n, \mathbf{v_t^n})$ with $\mathbf{w}_t^n = \mathfrak{m}(\mathbf{u_t^n})\mathbf{v_t^n}$, such that

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Basic idea: write everything in terms of $(u, \mathbf{w})$! Since $\mathbf{w} = \mathfrak{m}(\mathbf{u})\mathbf{v}$ we minimize

$$\mathcal{A}(u, \mathbf{w}) := \int_0^1 \int_{\mathbb{R}^d} A(u_t, \mathbf{w}_t)\,\mathrm{d}x\,\mathrm{d}t \quad \text{s.t.} \quad \partial_t u + \mathrm{div}\,\mathbf{w}_t = 0, \quad u\big|_{t=0,1} = u_{0,1}.$$

where $$\boxed{A(u, \mathbf{w}) := \frac{|\mathbf{w}|^2}{\mathfrak{m}(\mathbf{u})}}$$

Convexity (and l.s.c.) of the action requires a concave mobility

Lemma

The function

$$A : (u, \mathbf{w}) \in (0, +\infty) \times \mathbb{R}^d \to \frac{|\mathbf{w}|^2}{\mathfrak{m}(\mathbf{u})} \in [0, +\infty]$$

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A) $\mathfrak{m} : [0, +\infty) \to [0, +\infty)$ is concave and nondecreasing.
Model example: $\mathfrak{m}(\mathbf{u}) = \mathbf{u}^{\alpha}$, $0 \le \alpha \le 1$. In this case $A(\lambda u, \lambda \mathbf{w})$ is superlinear as $\lambda \uparrow +\infty$, except when $\mathbf{w} = 0$.

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B) $\mathfrak{m} : [0, M] \to [0, +\infty)$ is concave with $\mathfrak{m}(0) = \mathfrak{m}(M) = 0$.
Model example: $\mathfrak{m}(\mathbf{u}) = \mathbf{u}(\mathbf{M} - \mathbf{u})$. In this case $A(u, \mathbf{w}) = +\infty$ if $u > M$ and all the densities u are uniformly bounded.

A rigorous definition through convex functional of measures

To get weak* lower semicontinuity of $\mathcal{A}$, we extend it to

couples $(\boldsymbol{\rho}, \boldsymbol{\nu})$ *where* $\boldsymbol{\rho} \in \mathcal{M}_{\mathrm{loc}}(\mathbb{R}^d)$ *is a* **nonnegative Radon measure** *and* $\boldsymbol{\nu} \in \mathcal{M}_{\mathrm{loc}}(\mathbb{R}^d; \mathbb{R}^d)$ *is a* **Radon vector measure.**

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Moreover, *the function A is no more* $1-$*homogeneous* in the couple $(\rho, \boldsymbol{\nu})$, so that **the definition of $\mathcal{A}$ also depends from a reference measure $\boldsymbol{\gamma} \in \mathcal{M}_{\mathrm{loc}}(\mathbb{R}^d)$** (usually the Lebesgue measure, but not necessarily).

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Definition (The case of a sublinear mobility)

If $\rho \in \mathcal{M}_{\rm loc}(\mathbb{R}^d), \boldsymbol{\nu} \in \mathcal{M}_{\rm loc}(\mathbb{R}^d;\mathbb{R}^d)$ we set

$$\mathcal{A}(\rho, \boldsymbol{\nu}|\gamma) := \int_{\mathbb{R}^d} A\Big(\frac{\mathrm{d}\rho}{\mathrm{d}\gamma}, \frac{\mathrm{d}\boldsymbol{\nu}}{\mathrm{d}\gamma}\Big)\,\mathrm{d}\gamma$$

Given ρ_0, ρ_1 we have

$$\mathrm{W}^2_{\mathfrak{m},\gamma}(\rho_0,\rho_1) := \inf\Big\{\int_0^1 \mathcal{A}(\rho_t, \boldsymbol{\nu}_t)\,\mathrm{d}t \quad \text{s.t.} \quad \partial_t\rho + \operatorname{div}\boldsymbol{\nu} = 0, \quad \rho\big|_{t=0,1} = \rho_{0,1}\Big\}$$

We call $\mathcal{M}_{\mathfrak{m},\gamma}[\sigma]$ the collection of all measures at finite distance from σ.

[Dolbeault-Nazaret-S. '09, Lisini-Marigonda '10]

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Suppose that $\gamma^{\mathbf{n}} \rightharpoonup \gamma$, $\rho_i^n \rightharpoonup \rho_i$ *in* $\mathcal{M}_{\mathrm{loc}}(\mathbb{R}^d)$ *and* $\mathfrak{m}^{\mathbf{n}} \downarrow \mathfrak{m}$ *pointwise in* $[0, +\infty)$. *Then*

$$\liminf_{n\to+\infty} \mathrm{W}_{\mathfrak{m}^n,\gamma^n}(\rho_0^n, \rho_1^n) \geq \mathrm{W}_{\mathfrak{m},\gamma}(\rho_0, \rho_1).$$

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Simplest case: bounded Ω with $\mathfrak{m}$ defined on a bounded interval. In this case $W_{\mathfrak{m}}$ **induces the weak*-topology** on $L^\infty_+(\Omega)$.

Outline

1. Evolution PDE's with a gradient flow structure

2. The dynamical approach to weighted transport distances

3. **Basic tools for metric gradient flows: displacement convexity, variational approximation (JKO and WED schemes), flow interchange.**

Displacement convexity for weighted transport distances

A functional Φ is displacement convex if for every $\mathbf{u}_0, \mathbf{u}_1$ there exists a geodesic $\mathbf{u}_t$, $t \in [0,1]$, w.r.t. $\mathrm{W}_{\mathfrak{m}}$ connecting $\mathbf{u}_0$ to $\mathbf{u}_1$ such that

$$\mathrm{W}_{\mathfrak{m}}(\mathbf{u}_t, \mathbf{u}_s) = |t-s|\mathrm{W}_{\mathfrak{m}}(\mathbf{u}_0, \mathbf{u}_1), \qquad \Phi(\mathbf{u}_t) \le (1-t)\Phi(\mathbf{u}_0) + t\Phi(\mathbf{u}_1).$$

The functional generating the Heat equation is always displacement convex.

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Theorem (Generalized McCann condition [Carrillo-Lisini-S.-Slepcev '09])

The functional

$$\Phi(u) = \int F(u)\,\mathrm{d}x$$

is displacement convex in $\mathcal{M}_{\mathfrak{m}}(\Omega)$ *with respect to the distance* $\mathrm{W}_{\mathfrak{m}}$ *if*

$$r \mapsto \frac{H(r)}{\mathbf{m(r)^{1-1/d}}} \quad \text{is nonnegative and non decreasing in } (0,+\infty),$$

where

$$H(r) := \int_0^r F''(z)\mathfrak{m}(z)\mathfrak{m}'(z)\,\mathrm{d}z.$$

Displacement convexity for weighted transport distances

A functional Φ is displacement convex if for every $\mathbf{u}_0, \mathbf{u}_1$ there exists a geodesic $\mathbf{u}_t$, $t \in [0,1]$, w.r.t. $\mathrm{W}_{\mathfrak{m}}$ connecting $\mathbf{u}_0$ to $\mathbf{u}_1$ such that

$$\mathrm{W}_{\mathfrak{m}}(\mathbf{u}_t, \mathbf{u}_s) = |t-s|\mathrm{W}_{\mathfrak{m}}(\mathbf{u}_0, \mathbf{u}_1), \qquad \Phi(\mathbf{u}_t) \le (1-t)\Phi(\mathbf{u}_0) + t\Phi(\mathbf{u}_1).$$

Theorem (Generalized McCann condition [Carrillo-Lisini-S.-Slepcev '09])

The functional

$$\Phi(u) = \int F(u)\,\mathrm{d}x$$

is displacement convex in $\mathcal{M}_{\mathfrak{m}}(\Omega)$ *with respect to the distance* $\mathrm{W}_{\mathfrak{m}}$ *if*

$$r \mapsto \frac{H(r)}{\mathbf{m(r)^{1-1/d}}} \quad \text{is nonnegative and non decreasing in } (0,+\infty),$$

where

$$H(r) := \int_0^r F''(z)\mathfrak{m}(z)\mathfrak{m}'(z)\,\mathrm{d}z.$$

The functional generating the Heat equation is always displacement convex.

Weighted Energy-Dissipation (WED) approximation

Given $u_0 \in D(\Phi) \subset L^\infty_+(\Omega)$ and a relaxation parameter $\varepsilon > 0$ consider the space-time minimization of the WED functional

$$\mathfrak{I}_\varepsilon(u_0) := \min \Big\{ \int_0^\infty \frac{\mathrm{e}^{-t/\varepsilon}}{\varepsilon} \Big(\varepsilon \int_{\mathbb{R}^d} |\mathbf{v_t}|^2 \mathfrak{m}(\mathbf{u_t}) \,\mathrm{d}x + \Phi(u_t) \Big) \,\mathrm{d}t : \\ \partial_t u_t + \mathrm{div}\,\big(\mathfrak{m}(\mathbf{u_t})\mathbf{v_t}\big) = 0, \quad u(\cdot,0) = u_0 \Big\}$$

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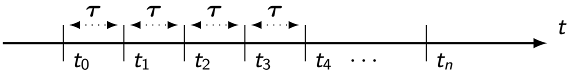
Theorem (Rossi-S.-Segatti-Stefanelli)

Assume that Φ is displacement convex w.r.t. $\mathrm{W}_\mathfrak{m}$ and has compact sublevels. Then the family of minimizers $\{u_\varepsilon\}$ of the WED functional is relatively compact and every limit point is a gradient flow of Φ.

The JKO-De Giorgi's Minimizing movement scheme

- Choose a partition of $(0, +\infty)$ of **step size** $\boldsymbol{\tau} > 0$



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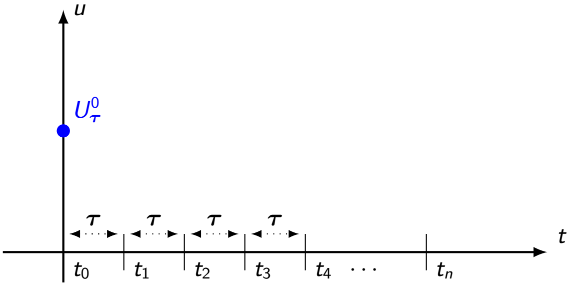

- Starting from $U_\tau^0 := \rho_0$ **find recursively** $U_\tau^n, \;\; n = 1, 2, \dots,$

$$\frac{U_\tau^n - U_\tau^{n-1}}{\tau} + \nabla\Phi(U_\tau^n) = 0$$

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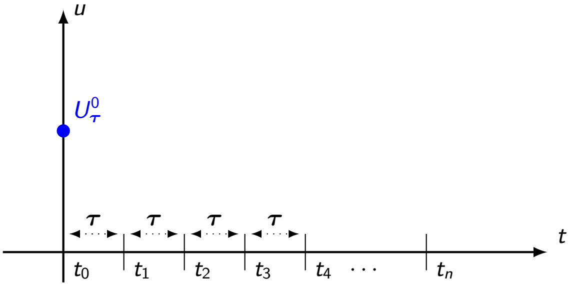

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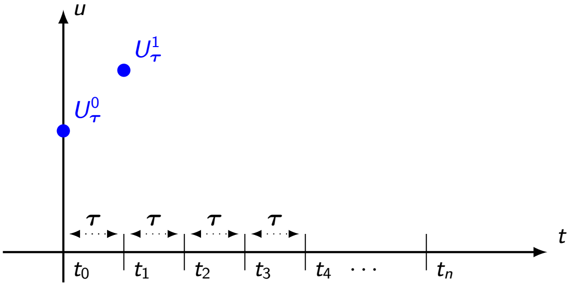

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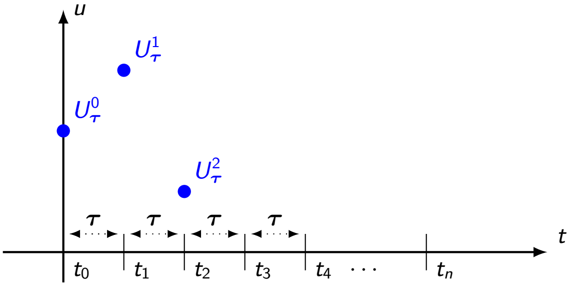

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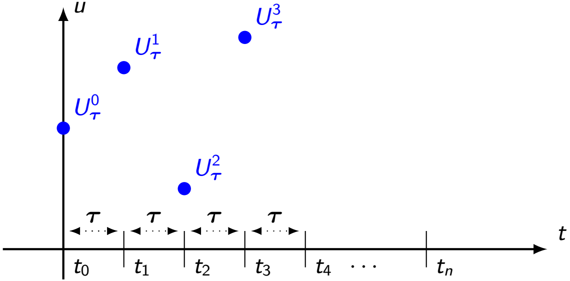

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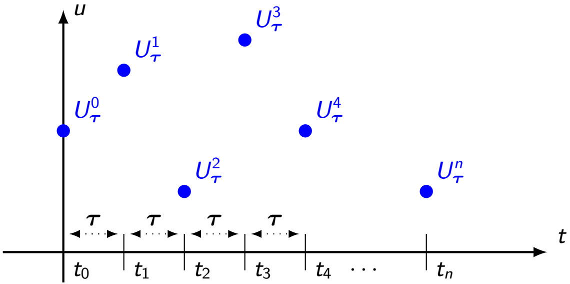

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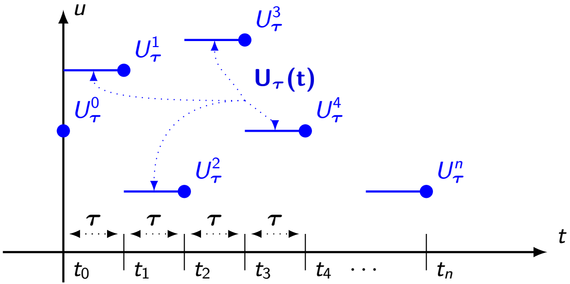

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- $\mathbf{U}_\tau$ is the **piecewise constant** interpolant of $\{U_\tau^n\}_n$.
  We look for **convergence results of** $\mathbf{U}_\tau$ **as** $\tau \downarrow 0$.

First variation along auxiliary flows

MAIN IDEA: take the first variation of the minimum problem

$$U_\tau^n \in \operatorname*{argmin}_V \frac{W^2(V, U_\tau^{n-1})}{2\tau} + \Phi(V)$$

along the gradient flow S^Ψ generated by other **"good" auxiliary functionals Ψ**.

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A Lyapunov-type estimate at the discrete level

Suppose that Ψ generates a flow $w_t = S_t^{\Psi}(w)$ satisfying a suitable metric formulation.

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$$\mathfrak{D}(\mathbf{w}) := \boxed{-}\frac{\mathrm{d}}{\mathrm{d}\varepsilon}\boldsymbol{\Phi}(\mathbf{S}_{\varepsilon}^{\boldsymbol{\Psi}}(\mathbf{w}))\Big|_{\varepsilon=0^+} = \limsup_{\varepsilon\downarrow 0} \frac{\boldsymbol{\Phi}(\mathbf{w}) - \boldsymbol{\Phi}(\mathbf{S}_{\varepsilon}^{\boldsymbol{\Psi}}(\mathbf{w}))}{\varepsilon}$$

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Theorem (Discrete flow-interchange estimate)

If $\mathbf{U}_\tau^{\mathbf{n}}$ *is a minimizer of* $V \mapsto \dfrac{W^2(V, \mathbf{U}_\tau^{\mathbf{n-1}})}{2\tau} + \boldsymbol{\Phi}(V)$ *then*

$$\boldsymbol{\Psi}(\mathbf{U}_\tau^{\mathbf{n}}) + \tau\,\mathfrak{D}(\mathbf{U}_\tau^{\mathbf{n}}) \le \boldsymbol{\Psi}(\mathbf{U}_\tau^{\mathbf{n-1}})$$

Auxiliary flow for the Cahn-Hilliard equation

A typical example in the case of the Cahn-Hilliard equation with mobility $\mathfrak{m}(u) = u(1-u)$ is given by the (displacement convex) entropy functional

$$\Psi(w) = \int_\Omega w \log w + (1-w)\log(1-w)\,dx$$

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In term of U_τ it corresponds to

$$\int_0^T\int_\Omega |D^2 U_\tau|^2\,dx\,dt \le C.$$

An example of convergence result

Assume that

$$P'(r) = \mathfrak{m}(\mathbf{r}) W''(r) \geq -C \quad \text{in } (0,1),$$

and the initial condition u_0 satisfies

$$0 \leq u_0 \leq 1, \quad \boldsymbol{\Phi}(u_0) = \int_\Omega \Big(\frac{1}{2} |\mathrm{D}u|^2 \, \mathrm{d}x + W(u_0) \Big) \, \mathrm{d}x$$

$\mathbf{u} \in C^0_w([0,+\infty); W^{1,2}(\Omega)) \cap L^2_{\mathrm{loc}}([0,+\infty); W^{2,2}(\mathbb{R}^d))$ *is a non-negative global solution of the weak formulation of the Cahn-Hilliard equation*

$$\iint \Big(\mathbf{u}\, \partial_t \zeta - \Delta \mathbf{u} \, \mathrm{div}\, \big(\mathfrak{m}(\mathbf{u}) \mathrm{D}\zeta \big) + P(\mathbf{u}) \Delta \zeta \Big) \, \mathrm{d}x\mathrm{d}t = 0,$$

for every test function $\zeta \in \mathrm{C}^\infty_c(\overline{\Omega} \times (0,\infty))$ *such that* $\mathrm{D}\zeta \cdot \mathbf{n} = 0$ *on* $\partial\Omega \times (0,\infty)$.

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Theorem

There exists an infinitesimal subsequence of time steps $\tau_k \downarrow 0$ such that

$$\mathbf{U}_{\tau_k} \to \mathbf{u} \quad \textit{pointwise in } L^2(\mathbb{R}^d) \textit{ and in } L^2(0,T;W^{1,2}(\mathbb{R}^d)) \quad \textit{as } k \uparrow \infty$$

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$$\mathbf{U}_{\tau_k} \to \mathbf{u} \quad \textit{pointwise in } L^2(\mathbb{R}^d) \textit{ and in } L^2(0,T;W^{1,2}(\mathbb{R}^d)) \quad \textit{as } k \uparrow \infty$$

$\mathbf{u} \in C^0_w([0,+\infty);W^{1,2}(\Omega)) \cap L^2_{\mathrm{loc}}([0,+\infty);W^{2,2}(\mathbb{R}^d))$ *is a non-negative global solution of the weak formulation of the Cahn-Hilliard equation*

$$\iint \Big(\mathbf{u}\,\partial_t\zeta - \Delta\mathbf{u}\ \mathrm{div}\,\big(\mathfrak{m}(\mathbf{u})\mathrm{D}\zeta\big) + P(\mathbf{u})\Delta\zeta\Big)\,\mathrm{d}x\mathrm{d}t = 0,$$

for every test function $\zeta \in \mathrm{C}^\infty_c(\overline{\Omega}\times(0,\infty))$ such that $\mathrm{D}\zeta\cdot\mathbf{n} = 0$ on $\partial\Omega\times(0,\infty)$.

Open problems

- More explicit characterizations of $W_{\mathfrak{m}}$ and of measures at finite $W_{\mathfrak{m}}$-distance.
- Develop a duality approach to the weighted distances and find a precise characterization of their geodesics. [Carliet-Nazaret-Cardaliaguet '12]. Curvature properties?
- Study the gradient flow of other integral functionals: potential and interaction energies do not behave well with respect to the weighted distances.
- What about non-concave mobilities?
- .....