A degenerate Cahn-Hilliard model as constrained Wasserstein gradient flow

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Existence of solutions to a non-local Cahn-Hilliard model with degenerate mobility is considered. The PDE is written as a gradient flow with respect to the $L^2$-Wasserstein metric for two components that are coupled by an incompressibility constraint. Approximating solutions are constructed by means of an implicit discretization in time and variational methods.

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1 The PDE system and its formal derivation

Degenerate Cahn-Hilliard system. We consider a mixture of two liquid phases of respective volume fractions $\rho(x), \eta(x) \in [0,1]$ on a spatial domain $\Omega \subset \mathbb{R}^n$, with $n \in \{1,2,3\}$. The dynamics is given by [1]

$$\partial_t \rho = \text{div}(\rho \nabla \phi), \quad \partial_t \eta = \text{div}(\eta \nabla \psi), \quad \phi - \psi = \Delta f(\rho) - \chi \rho, \quad \rho + \eta = 1, \quad (1)$$

where $f : [0,1] \to \mathbb{R}$ is either $f(r) = r$ or $f(r) = 2 \arcsin(\sqrt{r})$, and $\phi, \psi : \Omega \to \mathbb{R}$ are time-dependent auxiliary potentials. Below, we show how (1) is derived from variational principles. And we indicate the proof for existence of weak solutions.

Energy functional. Let $X := \{ \tilde{\rho} = (\rho, \eta) : \Omega \to [0,1]^2 \mid \int_\Omega \rho \, dx = m_1, \int_\Omega \eta \, dx = m_2 \},$ where $m_1, m_2 > 0$ are fixed, with $m_1 + m_2 = |\Omega|$. Define the energy functional $E : X \to \mathbb{R}_{\geq 0} \cup \{+\infty\}$ by

$$E(\tilde{\rho}) = \int_\Omega \left( |\nabla f(\rho)|^2 + |\nabla f(\eta)|^2 \right) \, dx + \frac{\chi}{2} \int_\Omega \rho \eta \, dx. \quad (2)$$

The two choices $f(r) = r$ and $f(r) = 2 \arcsin(\sqrt{r})$ correspond to, respectively,

$$|\nabla f(\rho)|^2 = |\nabla \rho|^2 \quad \text{and} \quad |\nabla f(\eta)|^2 = \frac{|\nabla \rho|^2}{\rho(1 - \rho)} \quad (3)$$

The first choice leads to the most classical Cahn-Hilliard model; for the second choice, $E$ is the famous Flory-Huggins-deGennes energy [2]. Notice that in both cases, the integral involving the squared gradients is convex in $\tilde{\rho}$, whereas the integral involving $\rho \eta$ is not. To incorporate the volume constraint, let the functional $E : X \to \mathbb{R}_{\geq 0} \cup \{+\infty\}$ be defined such that $E(\tilde{\rho}) = E(\bar{\rho})$ if $\rho + \eta = 1$ a.e. in $\Omega$, and $E(\tilde{\rho}) = +\infty$ otherwise.

Wasserstein metric. The Wasserstein metric $W$ on probability densities on $\Omega$ can be defined in two ways, referred to as primal and dual formulation of the optimal transport problem:

$$W(\rho_0, \rho_1)^2 = \inf \left\{ \int_\Omega |v|^2 \rho_1 \, dx \mid (\text{id} + v) \# \rho_1 = \rho_0 \right\} \quad (4)$$

$$= \sup \left\{ \int_\Omega (\phi \rho_0 + \phi \rho_1) \, dx \mid \phi(x) + \phi(y) \leq \frac{1}{2} |x - y|^2 \right\}. \quad (5)$$

We shall need both formulations in the sequel. In the primal problem, one minimizes the kinetic energy over all velocity fields $v : \Omega \to \mathbb{R}^n$ which are such that if all “mass particles” of $\rho_1$ are moved along $v$, then the resulting density is $\rho_0$. In the dual problem, one optimizes over all Kantorovich potentials $\phi, \tilde{\phi} : \Omega \to \mathbb{R}$ that can be understood as optimal prices for transshipment. The optimizers are attained in both problems, and are related in the sense that $\nu_{\text{opt}} = \nabla \phi_{\text{opt}}$.

The natural extension of $W$ to two-component densities $\tilde{\rho} \in X$ is given by

$$W(\tilde{\rho}_0, \tilde{\rho}_1)^2 = W(\rho_0, \rho_1)^2 + W(\eta_0, \eta_1)^2.$$ 

$W$ is again a metric, and inherits the associated primal and dual formulations.

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Gradient flow equation. There is an infinitesimal “metric tensor” $g$ associated to $W$, whose shape can be derived by combining the primal and dual formulations: if $\bar{p} = (p, q)$ is a tangent vector at $\bar{p}$, then

$$g[\bar{p}]^2 = \int_\Omega (|\nabla \phi|^2 p + |\nabla \psi|^2 q) \, dx,$$

where $\phi, \psi$ satisfy $p = \text{div}(\rho \nabla \phi)$, $q = \text{div}(\eta \nabla \psi)$.

Formally, a curve $\bar{p}(\cdot) : [0, \infty) \to X$ is a solution to the gradient flow of $\mathcal{E}$ w.r.t. $W$ if $\dot{\bar{p}}_t[\partial_t \bar{p}_t, \bar{p}_t] = -D \mathcal{E}(\bar{p}_t)[\bar{p}_t]$ holds for any tangent vector $\dot{\bar{p}}$ at $\bar{p}_t$. The differential on the right side is undefined unless $\dot{\bar{p}}$ preserves the volume constraint, that is $q = -p$. In that case, we have for the solutions $(\partial_t \bar{p}_t, \psi_t)$ to $\text{div}(\rho_t \nabla \phi_t) = \partial_t \rho_t = -\partial_t \eta_t = -\text{div}(\eta_t \nabla \psi)$ the relation

$$\int (\phi_t - \psi_t) p \, dx = \int |\Delta f(p_t) - \chi p_t| p \, dx.$$

This produces the coupled system (1).

2 Existence of solutions

Our main result [3] is:

**Theorem 2.1** Given $\bar{p}_0 \in X$ with $\mathcal{E}(\bar{p}_0) < \infty$, then there exists at least one weak solution $(\bar{p}_t)_{t \geq 0}$ to (1).

First, we construct a time-discrete (time step $\tau > 0$) approximation $(\bar{p}^\tau_n)_n$ of $\bar{p}_t$ via:

$$\bar{p}^\tau_n \in \arg \min_{\bar{p} \in X} \mathcal{E}_\tau(\bar{p}; \bar{p}^{n-1}) \quad \text{where} \quad \mathcal{E}_\tau(\bar{p}; \bar{p}') := \frac{1}{2\tau} W(\bar{p}, \bar{p}')^2 + \mathcal{E}(\bar{p}).$$

Summing the inequalities $\mathcal{E}_\tau(\bar{p}^\tau_n; \bar{p}^{n-1}) \leq \mathcal{E}_\tau(\bar{p}^{n-1}; \bar{p}^{n-2})$, one obtains:

**Lemma 2.2** The minimizers $\bar{p}^\tau_n$ are well-defined for each $n$, and

$$\mathcal{E}(\bar{p}_n^\tau) \leq \mathcal{E}(\bar{p}_n^{n-1}) \leq \sum_{k=1}^N \left( \frac{W(\bar{p}_n^\tau, \bar{p}^{n-1})}{\tau} \right)^2 \leq C N \tau.$$

The first estimate above provides compactness in space, the second compactness in time. By an Arzelà-Ascoli argument, it follows that any reasonable interpolation of $(\bar{p}^\tau_n)_n$ in time converges as $\tau \to 0$ (at least along a subsequence) to a Hölder continuous limit curve $\bar{p}_* : [0, \infty) \to X$. It remains to show that $\bar{p}_*$ (with appropriate $\phi$ and $\psi$) is a weak solution to (1).

Time-discrete versions of the continuity equations for $\rho$ and $\eta$ in (1) are a consequence of the primal formulation (4) of the optimal transport problem: with $v^\rho_n = \nabla \phi^\rho_n$ and $w^\psi_n = \nabla \psi^\rho_n$ being the optimal vector fields for the passage from $\bar{p}^{n-1}_\tau$ to $\bar{p}^\tau_n$, we conclude from $(\text{id} + v^\rho_n) \# \rho^\tau_n = \rho^{n-1}_\tau$ that

$$\int_\Omega \frac{\rho^\tau_n - \rho^{n-1}_\tau}{\tau} \theta \, dx = \int_\Omega \nabla \theta \cdot \nabla v^\rho_n \rho^\tau_n \, dx + O(\tau) \quad \text{for each } \theta \in C^\infty_c(\Omega),$$

and likewise for $\eta^\tau_n$. To derive the Euler-Lagrange equation involving $\phi - \psi$ in (1), we use the dual formulation (5) of optimal transport, and compare

$$\mathcal{E}_\tau(\bar{p}^\tau_n; \bar{p}^{n-1}) = \frac{1}{2\tau} \left[ \int (\phi^\rho_n \rho^\tau_n + \phi^\rho_n \rho^{n-1}_\tau) \, dx + \int (\psi^\rho_n \eta^\tau_n + \psi^\rho_n \eta^{n-1}_\tau) \, dx \right] + \mathcal{E}(\bar{p}^\tau_n)$$

from above with $\mathcal{E}_\tau(\bar{p}; \bar{p}^{n-1})$ for some variation $\bar{p}'$ of $\bar{p}^\tau_n$, and from below with the same expression as above, in which $\phi^\rho_n, \psi^\rho_n$ are replaced by the respective potentials $\phi', \psi'$ for $\bar{p}'$. This provides a rigorous justification of the formal calculation leading to (6) above. Finally, to pass to the limit in the discrete system, we justify the following a priori estimate for the time-discrete approximation:

$$-\frac{d}{dt} \int_\Omega (\rho \log \rho + \eta \log \eta) \, dx \geq c \int_\Omega (|\Delta f(\rho)|^2 + |\Delta f(\eta)|^2) \, dx.$$

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