THE CAHN-HILLIARD EQUATION WITH A LOGARITHMIC POTENTIAL AND DYNAMIC BOUNDARY CONDITIONS

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Cahn-Hilliard system :

$$\begin{aligned} &\frac{\partial u}{\partial t} = \kappa \Delta w, \ \kappa > 0 \\ &w = -\alpha \Delta u + f(u), \ \alpha > 0 \end{aligned}$$

Equivalently :

$$\frac{\partial u}{\partial t} + \alpha\kappa\Delta^2 u - \kappa\Delta f(u) = 0$$

Describes the phase separation process in a binary alloy : spinodal decomposition, coarsening

u : order parameter
w : chemical potential
κ : mobility
α : related to the surface tension at the interface

f : derivative of a double-well potential F

Typical choice :

$$F(s) = \frac{1}{4}(s^2-1)^2$$
$$f(s) = s^3 - s$$

Thermodynamically relevant potential :

$$F(s) = -\theta_0 s^2 + \theta_1((1+s)\ln(1+s)$$
$$+(1-s)\ln(1-s))$$
$$f(s) = -2\theta_0 s + \theta_1 \ln\frac{1+s}{1-s}$$
$$s \in (-1,1),\ 0 < \theta_1 < \theta_0$$

Derivation of the Cahn-Hilliard system :

Mass balance : $\frac{\partial u}{\partial t} = -\text{div}h$

h : mass flux

Constitutive equation : $h = -\kappa\nabla w$

Ginzburg-Landau free energy : $\Psi_{\text{GL}}(u, \nabla u) = \int_{\Omega}(\frac{\alpha}{2}|\nabla u|^2 + F(u))dx$

$\Omega \subset R^N,\ N \leq 3$: domain occupied by the material

Usual definition of w : derivative of Ψ_{GL} w.r.t. u

$\longrightarrow$ No longer valid

New definition : variational derivative of Ψ_{GL} w.r.t. u

$\longrightarrow w = -\alpha\Delta u + F(u)$

Usual boundary conditions :

$$\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma$$
$$\frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma$$

$\Gamma = \partial\Omega$
ν : unit outer normal vector

$\longrightarrow$ Mass conservation : $\frac{d}{dt}\int_\Omega u dx = 0$

Equivalently :

$$\frac{\partial u}{\partial \nu} = \frac{\partial \Delta u}{\partial \nu} = 0 \text{ on } \Gamma$$

Regular potentials :

• Well-posedness, regularity : C.M. Elliott-S. Zheng, B. Nicolaenko-B. Scheurer, D. Li-C. Zhong, ...

• Existence of finite-dimensional attractors : B. Nicolaenko-B. Scheurer-R. Temam, D. Li-C. Zhong, ...

• Convergence of solutions to steady states : S. Zheng, P. Rybka-K.-H. Hoffmann

Logarithmic (singular) potentials :

Main difficulty : prove that u remains in $(-1, 1)$

Remark : Not true for regular potentials

• Well-posedness, regularity : C.M. Elliott-S. Luckhaus, C.M. Elliott-H. Garcke, A. Debussche-L. Dettori, A. Miranville-S. Zelik

• Existence of finite-dimensional attractors : A. Debussche-L. Dettori, A. Miranville-S. Zelik

• Convergence of solutions to steady states : H. Abels-M. Wilke

Dynamic boundary conditions :

Influence of the walls for confined systems

Mainly studied for polymer mixtures

Technological applications

Problem : define the boundary conditions (we need 2 boundary conditions)

First boundary condition : no mass flux at the boundary :

$$\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma$$

$\rightarrow$ Bulk mass conservation : $\frac{d}{dt} \int_\Omega u dx = 0$

Second boundary condition : we consider, in addition to the Ginzburg-Landau free energy

$$\Psi_{\mathrm{GL}}(u, \nabla u) = \int_{\Omega} (\frac{\alpha}{2} |\nabla u|^2 + F(u)) dx$$

the surface free energy

$$\Psi_{\Gamma}(u, \nabla u) = \int_{\Gamma} (\frac{\alpha_{\Gamma}}{2} |\nabla_{\Gamma} u|^2 + G(u)) dx$$

$\alpha_{\Gamma} > 0$
∇_{Γ} : surface gradient

Original surface potential : $G(s) = \frac{1}{2} a_{\Gamma} s^2 - b_{\Gamma} s$

$a_{\Gamma} > 0$: accounts for a modification of the effective interaction between the components
b_{Γ} : characterizes the preferential attraction of one of the components by the walls

Total energy : $\Psi = \Psi_{\mathrm{GL}} + \Psi_\Gamma$

The system tends to minimize the excess surface energy :

$$\frac{1}{d}\frac{\partial u}{\partial t} - \alpha_\Gamma \Delta_\Gamma u + g(u) + \alpha \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma$$

$d > 0$: relaxation parameter
Δ_Γ : Laplace-Beltrami operator
$g = G'$

$\rightarrow$ Dynamic boundary condition

Different approach : G.R. Goldstein-A. Miranville-G. Schimperna

Total mass conservation : $\frac{d}{dt}(\int_\Omega u dx + \int_\Gamma u d\sigma) = 0$

$\rightarrow \frac{\partial u}{\partial t} = \beta_\Gamma \Delta_\Gamma w - \kappa \frac{\partial w}{\partial \nu}$ on Γ, $\beta_\Gamma \geq 0$

Second boundary condition : w is a variational derivative of the total free energy Ψ w.r.t. u

$\rightarrow w = -\alpha_\Gamma \Delta_\Gamma u + g(u) + \alpha \frac{\partial u}{\partial \nu}$ on Γ

Regular potentials : the system is well understood

Contributors : R. Chill, C.G. Gal, E. Fašangová, A. Miranville, J. Pruess, R. Racke, H. Wu, S. Zelik, S. Zheng, ...

Singular potentials : more complicated and less understood

First existence and uniqueness result : G. Gilardi-A. Miranville-G. Schimperna

For f singular and g regular : sign assumptions on g near the singular points of f :

$$g(1) > 0, \; g(-1) < 0$$

Forces the order parameter to stay away from ± 1 on Γ

Question :

• What happens when the sign conditions are not satisfied ?

Nonexistence of classical solutions :

When the sign conditions are not satisfied, we can have nonexistence of classical solutions

We consider the scalar ODE

$$\begin{aligned} & y'' - f(y) = 0,\ x \in (-1,1) \\ & y'(\pm 1) = K > 0 \end{aligned}$$

Assumptions :

• f is singular at ± 1
• $F(\pm 1) < +\infty$ $(F' = f)$
• f is odd

Satisfied by the usual logarithmic potentials

When K is small : existence and uniqueness of a solution which is separated from the singular values ($\|y\|_{L^\infty(-1,1)} < 1$) and is odd

Standard interior regularity estimates yield

$$|y'(x)| \leq c_0,\ |y(x)| \leq 1 - \delta$$

$x \in (-\frac{1}{2}, \frac{1}{2})$, $\delta > 0$, c_0 independent of K

Multiply the equation by y' and integrate over $(0, 1)$:

$$|\frac{1}{2}K^2 - F(y(1))| \leq c_1$$

c_1 (and $F(\pm 1)$) independent of K

This inequality cannot hold when K is large

$\rightarrow$ We do not have a classical solution

Since y is odd, the ODE can be rewritten as

$$y'' - f(y) = < y'' - f(y) >$$

$< . > = \frac{1}{\mathrm{Vol}(\cdot)} \int_\Omega .dx$

$\rightarrow$ 1-D stationary Cahn-Hilliard system with dynamic BCs

Convergence of a sequence of solutions to regularized problems :

$$\begin{aligned}
&\frac{\partial u}{\partial t} = \Delta w \\
&w = -\Delta u + f_0(u) + \lambda u,\ \lambda \in R \\
&\frac{\partial w}{\partial \nu} = 0 \text{ on } \Gamma \\
&\frac{\partial \psi}{\partial t} - \Delta_\Gamma \psi + g_0(\psi) + \psi + \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma \\
&\psi = u|_\Gamma
\end{aligned}$$

$f(s) = f_0(s) + \lambda s,\ g(s) = g_0(s) + s$

Assumptions :

- $f_0 \in \mathcal{C}^2(-1,1),\ f_0(0) = 0$
- $\lim_{s\to\pm 1} f_0(s) = \pm\infty,\ \lim_{s\to\pm 1} f_0'(s) = +\infty$
- $f_0' \geq 0,\ \mathrm{sgn}(s) f_0''(s) \geq 0$
- $g_0 \in \mathcal{C}^2(R),\ \|g_0\|_{\mathcal{C}^2(R)} \leq c$

Regularized potential :

$$
\begin{aligned}
&f_{0,n}(s) = f_0(s),\ |s| \leq 1 - \tfrac{1}{n} \\
&f_{0,n}(s) = f_0(1 - \tfrac{1}{n}) + f_0'(1 - \tfrac{1}{n})(s - 1 + \tfrac{1}{n}) \\
&s > 1 - \tfrac{1}{n} \\
&f_{0,n}(s) = f_0(-1 + \tfrac{1}{n}) + f_0'(-1 + \tfrac{1}{n})(s + 1 - \tfrac{1}{n}) \\
&s < -1 + \tfrac{1}{n}
\end{aligned}
$$

Regularized problem : f_0 replaced by $f_{0,n}$

Existence and uniqueness of the solution u_n to the regularized problem

Satisfies, for n large enough

$$\|u_n(t)\|^2_{\mathcal{C}^\alpha(\Omega)} + \|u_n(t)\|^2_{H^2(\Gamma)} + \|u_n(t)\|^2_{H^2(\Omega_\epsilon)} + \|u_n(t)\|^2_{H^1(\Omega)} +$$
$$\|\frac{\partial u_n}{\partial t}(t)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(t)\|^2_{L^2(\Gamma)} +$$
$$\|\nabla D_\tau u_n(t)\|^2_{L^2(\Omega)^{2N}} + \|f_{0,n}(u_n(t))\|_{L^1(\Omega)} +$$
$$\int_t^{t+1}(\|\frac{\partial u_n}{\partial t}(s)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(s)\|^2_{L^2(\Gamma)})ds \leq$$
$$ce^{-\beta t}(1 + \|u_n(0)\|^2_{H^1(\Omega)} + \|u_n(0)\|^2_{H^1(\Gamma)} +$$
$$\|\frac{\partial u_n}{\partial t}(0)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(0)\|^2_{L^2(\Gamma)})^2 + c'$$

$\Omega_\epsilon = \{x \in \Omega,\ d(x, \Gamma) > \epsilon\},\ \epsilon > 0$
$D_\tau u_n = \nabla u_n - \frac{\partial u_n}{\partial \nu}\nu$
$\alpha > 0,\ \beta > 0,\ c,\ c'$ independent of n

Remark : Actually, $u_n(t) \in H^2(\Omega)$, but this regularity does not pass to the limit

Smoothing property :

$$\|\frac{\partial u_n}{\partial t}(t)\|^2_{H^{-1}(\Omega)} + \|\frac{\partial u_n}{\partial t}(t)\|^2_{L^2(\Gamma)} \leq$$
$$\frac{c}{t}(1 + \|u_n(0) - < u_n(0) > \|^2_{H^{-1}(\Omega)} + \|u_n(0)\|^2_{L^2(\Gamma)})$$

$t \in (0,1],\ c$ independent of n

Lipschitz estimate :

$$\|u_1(t) - u_2(t)\|_{H^{-1}(\Omega)} +$$
$$\|u_1(t) - u_2(t)\|_{L^2(\Gamma)} \leq$$
$$ce^{c't}(\|u_1(0) - u_2(0)\|_{H^{-1}(\Omega)} +$$
$$\|u_1(0) - u_2(0)\|_{L^2(\Gamma)})$$
$$< u_1(0) > = < u_2(0) > = m,\ t \geq 0$$

$c,\ c'$ independent of $t,\ n,\ u_1,\ u_2$

u_n converges to some function u

We wish to call u the "generalized" solution to the singular problem

Variational solutions :

We set

$$B(u,v) = (\nabla u, \nabla v)_\Omega + \lambda (u,v)_\Omega + \\ + L((-\Delta)^{-1}\overline{u}, \overline{v})_\Omega + (\nabla_\Gamma u, \nabla_\Gamma v)_\Gamma$$

$u,\ v \in H^1(\Omega) \otimes H^1(\Gamma) = \{w,\ w \in H^1(\Omega), w|_\Gamma \in H^1(\Gamma)\}$

$L > 0$ chosen s.t.

$$\|\nabla u\|^2_{L^2(\Omega)^3} + \lambda \|u\|^2_{L^2(\Omega)} + L\|u\|^2_{H^{-1}(\Omega)} \geq \\ \frac{1}{2}\|u\|^2_{H^1(\Omega)},\ u \in H^1(\Omega),\ <u>=0$$

$\overline{u} = u - <u>$

$(.,.)_\Omega$, $(.,.)_\Gamma$: scalar products in $L^2(\Omega)$ and $L^2(\Gamma)$

We rewrite the problem as

$$\begin{aligned}
&(-\Delta)^{-1}\frac{\partial u}{\partial t} - \Delta u + \\
&f_0(u) + \lambda u - < w >= 0 \\
&w = -\Delta u + f_0(u) + \lambda u \\
&\frac{\partial \psi}{\partial t} - \Delta_\Gamma \psi + g(\psi) + \frac{\partial u}{\partial \nu} = 0 \text{ on } \Gamma \\
&\psi = u|_\Gamma \\
&u|_{t=0} = u_0,\ \psi|_{t=0} = \psi_0
\end{aligned}$$

We multiply the first equation by $u - v$, $v = v(x)$ s.t.

$$< u(t) - v >= 0,\ t \geq 0 :$$

$$\begin{aligned}
&((-\Delta)^{-1}\frac{\partial u}{\partial t}, u - v)_\Omega + (\frac{\partial u}{\partial t}, u - v)_\Gamma + \\
&B(u, u - v) + (f_0(u), u - v)_\Omega = \\
&L(u, (-\Delta)^{-1}(u - v))_\Omega - (g(u), u - v)_\Gamma
\end{aligned}$$

Positivity of B and monotonicity of f_0 :

$$((-\Delta)^{-1}\frac{\partial u}{\partial t}, u-v)_\Omega + (\frac{\partial u}{\partial t}, u-v)_\Gamma +$$
$$B(v, u-v) + (f_0(v), u-v)_\Omega \leq$$
$$L(u, (-\Delta)^{-1}(u-v))_\Omega - (g(u), u-v)_\Gamma$$

Variational inequality (VI)

We set

$$\Phi = \{(u,\psi) \in L^\infty(\Omega) \times L^\infty(\Gamma),$$
$$\|u\|_{L^\infty(\Omega)} \leq 1,\ \|\psi\|_{L^\infty(\Gamma)} \leq 1\}$$

Definition : Let $(u_0, \psi_0) \in \Phi$. Then, (u, ψ) is a variational solution if

(i) $u(t)|_\Gamma = \psi(t)$ a.e. $t > 0$, $u(0) = u_0$, $\psi(0) = \psi_0$;

(ii) $-1 < u(t, x) < 1$ a.e. $(t, x) \in R^+ \times \Omega$;

(iii) $(u, \psi) \in \mathcal{C}([0, +\infty); H^{-1}(\Omega) \times L^2(\Gamma)) \cap L^2(0, T; H^1(\Omega) \times H^1(\Gamma))$, $T > 0$;

(iv) $f(u) \in L^1((0, T) \times \Omega)$, $T > 0$;

(v) $(\frac{\partial u}{\partial t}, \frac{\partial \psi}{\partial t}) \in L^2(\tau, T; H^{-1}(\Omega) \times L^2(\Gamma))$, $T > \tau > 0$;

(vi) $< u(t) >=< u_0 >$, $t \geq 0$;

(vii) the variational inequality (VI) is satisfied for a.e. $t > 0$ and every test function $v = v(x)$ s.t. $v \in H^1(\Omega) \otimes H^1(\Gamma)$, $f(v) \in L^1(\Omega)$, $< v >=< u_0 >$.

Remark : $u(t)|_\Gamma = \psi(t)$ only for $t > 0$

• A variational solution, if it exists is unique

• $\forall (u_0, \psi_0) \in \Phi$, $\exists$ a variational solution and $(u_n, \psi_n = u_n|_\Gamma)$ converges (for a subsequence) to a variational solution

• The variational solutions satisfy the a priori estimates mentioned earlier

• The variational solutions satisfy the smoothing and Lipschitz properties

• A variational solution does not necessarily solve the equations in the usual sense :

It satisfies the bulk equation

It does not necessarily satisfy the dynamic boundary condition

Existence of classical solutions :

Related to the H^2-regularity and the separation from the singularities of f_0

Theorem : Let (u, ψ) be a variational solution and set, for $\delta > 0$ and $T > 0$,

$$\Omega_\delta(T) = \{x \in \Omega,\ |u(T,x)| < 1 - \delta\}.$$

Then, $u(T) \in H^2(\Omega_\delta(T))$ and

$$\|u(T)\|_{H^2(\Omega_\delta(T))} \leq Q_{\delta,T},$$

where $Q_{\delta,T}$ is independent of u.

Consequence : if

$$|u(t,x)| < 1 \text{ a.e. } (t,x) \in R^+ \times \Gamma$$

then u is a classical solution

$\rightarrow$ The existence of classical solutions is related to the separation property on the boundary

True if f_0 has sufficiently strong singularities

Theorem : We assume that

$$\lim_{s \to \pm 1} F_0(s) = +\infty, \ F_0' = f_0.$$

Then, the separation property on the boundary holds and a variational solution is a classical one.

True if f_0 behaves like $\frac{s}{(1-s^2)^p}$, $p > 1$

Not true for logarithmic potentials

In that case, we can have $|u(t,x)| = 1$ on a set with nonzero measure on the boundary (possibly, on the whole boundary)

Theorem : We assume that

$$\pm g(\pm 1) > 0.$$

Then, a variational solution is a classical one.

Existence of finite-dimensional attractors :

Conservation of the total mass ($< u >$) : we restrict ourselves to

$$\Phi_m = \{(u,\psi) \in \Phi,\ < u >= m\},\ m \in (-1,1)$$

Theorem : For every $m \in (-1,1)$, the semigroup $S(t)$ acting on Φ_m possesses the finite-dimensional global attractor $\mathcal{A}_m$ (in $H^{-1}(\Omega) \times L^2(\Gamma)$) which is bounded in $\mathcal{C}^\alpha(\Omega) \times \mathcal{C}^\alpha(\Gamma)$, $0 < \alpha < \frac{1}{4}$.

Global attractor : unique compact set of Φ_m which is invariant ($S(t)\mathcal{A}_m = \mathcal{A}_m,\ t \geq 0$) and attracts all bounded sets of initial data

Suitable object in view of the study of the asymptotic behavior of the system (smallest closed set enjoying the attraction property)

Finite dimensionality : the reduced dynamics can be described by a finite number of parameters

Existence of the global attractor : follows from classical results

Finite-dimensionality : construction of an exponential attractor

Exponential attractor : compact and positively invariant $(S(t)\mathcal{M}_m \subset \mathcal{M}_m,\ t \geq 0)$ set which contains the global attractor and has finite fractal dimension

We need some (asymptotically) compact smoothing property on the difference of 2 solutions

We have

$$\|u_1(t) - u_2(t)\|^2_{\Phi^{\mathrm{w}}} \leq ce^{-\beta t}\|u_1(0) - u_2(0)\|^2_{\Phi^{\mathrm{w}}} + c' \int_0^t \|\theta(u_1(s) - u_2(s))\|^2_{L^2(\Omega)} ds$$

$\beta > 0$, θ : smooth cut-off function

$\Phi^{\mathrm{w}} = H^{-1}(\Omega) \times L^2(\Gamma)$

$\rightarrow$ Contraction, up to $\|\theta(u_1 - u_2)\|_{L^2(0,t;L^2(\Omega))}$

Compactness : We work on spaces of trajectories and use the compactness of

$$L^2(0,t;H^1(\Omega)) \cap H^1(0,t;H^{-3}(\Omega)) \subset L^2(0,t;L^2(\Omega))$$

We have

$$\|\frac{\partial}{\partial t}[\theta(u_1 - u_2)]\|^2_{L^2(0,t;H^{-3}(\Omega))} + \|\theta(u_1 - u_2)\|^2_{L^2(0,t;H^1(\Omega))} \leq ce^{c't}\|u_1(0) - u_2(0)\|^2_{H^{-1}(\Omega)\cap L^2(\Gamma)}$$

$u_1(0), u_2(0) \in B_{H^{-1}(\Omega)\cap L^2(\Gamma)}(u_0, \epsilon)$, $\epsilon > 0$ small