The Cahn-Hilliard equation

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The Cahn-Hilliard equation :

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 (in general : rescaled density of atoms taking values between -1 and 1)
w : chemical potential
κ : mobility
α : related to the surface tension at the interface

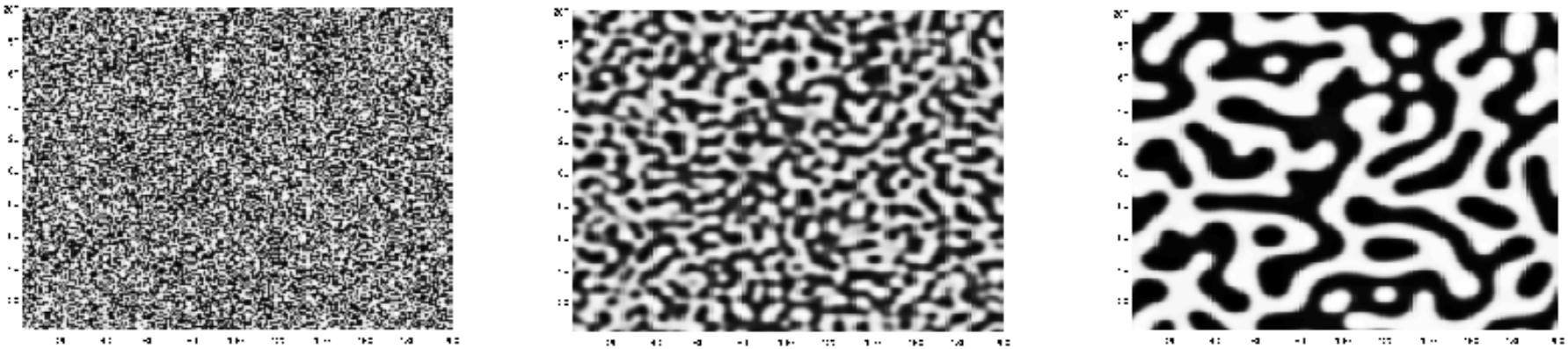


Figure – Spinodal decomposition, coarsening

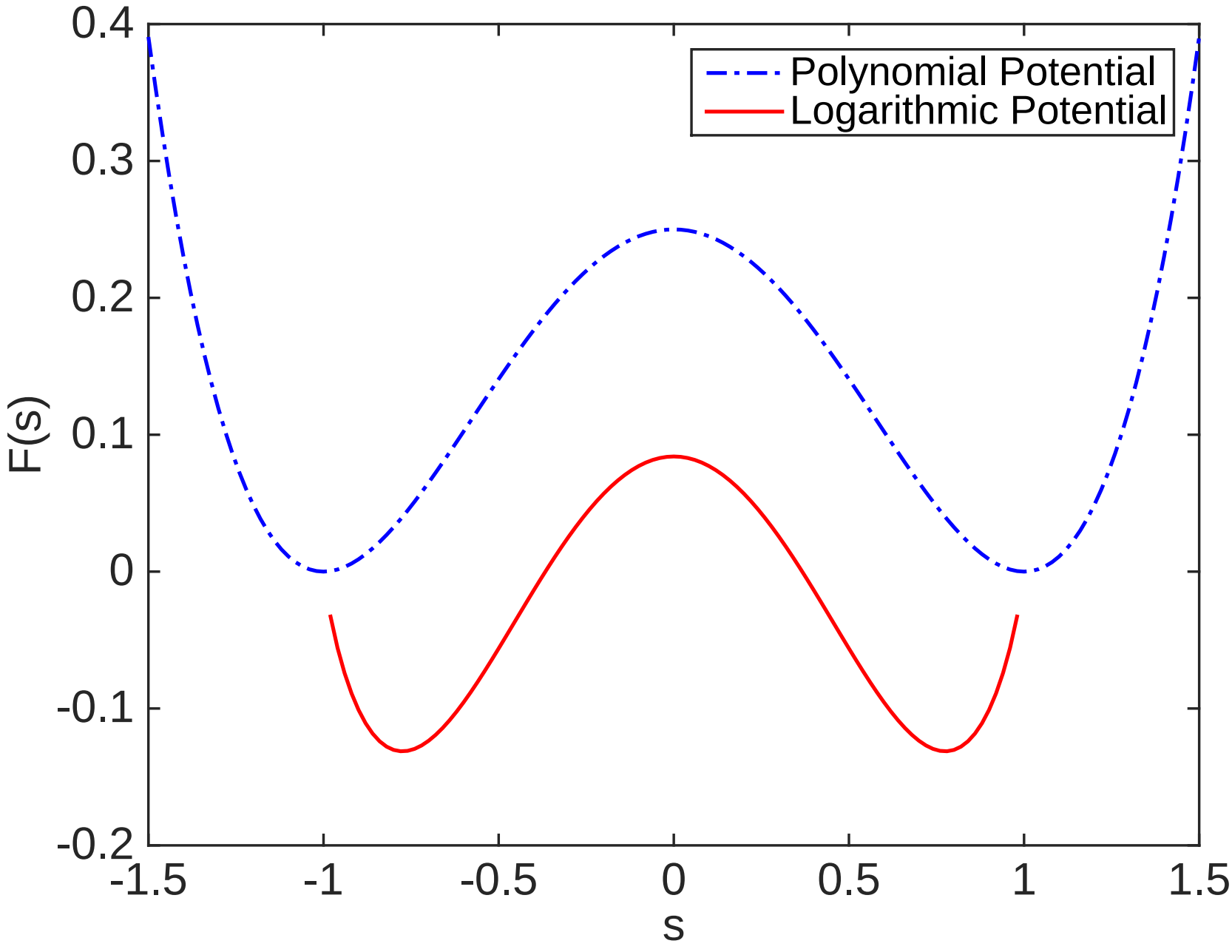
f : derivative of a double-well potential F

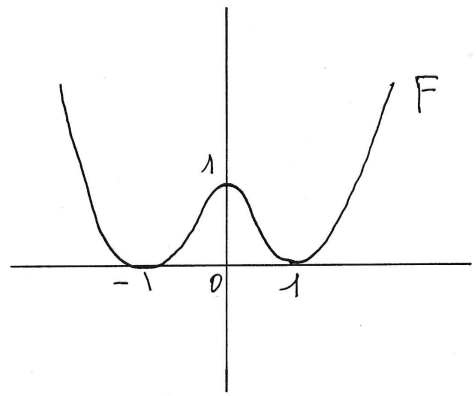
Typical choice :

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

Thermodynamically relevant potential :

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


Polynomial Potential
Logarithmic Potential
F(s)
s
0.4
0.3
0.2
0.1
0
-0.1
-0.2
-1.5
-1
-0.5
0
0.5
1
1.5


F
1
-1
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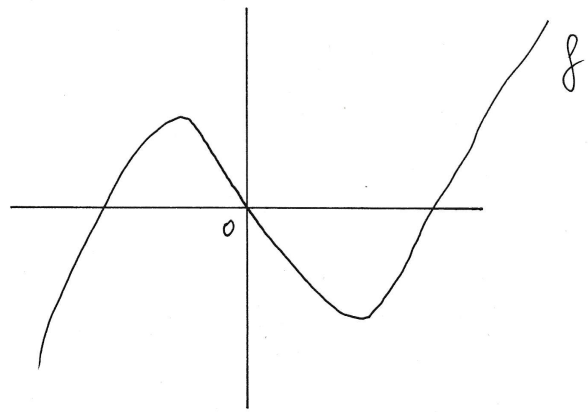
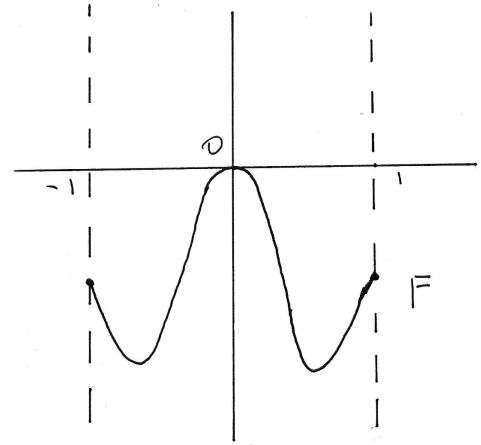
1


g
0


0
-1
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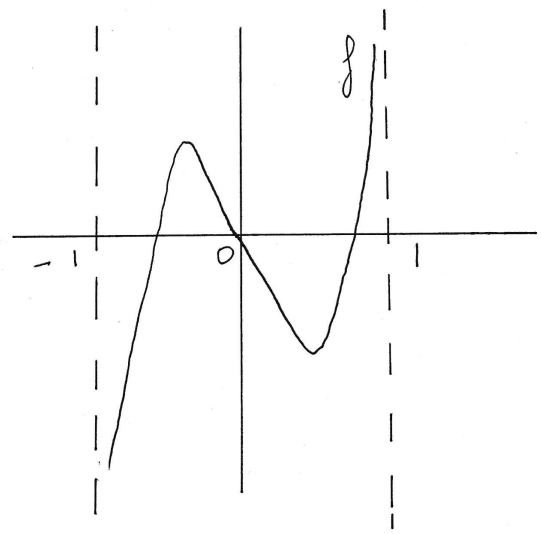
F


f
-1
0
1

Remark : κ should more generally depend on u and degenerate :

$$\frac{\partial u}{\partial t} = \mathrm{div}(\kappa(u)\nabla w)$$

$\kappa(s) = 1 - s^2$
Restricts the diffusion process to the interfacial region
Is observed when the movements of atoms are confined to this region

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

Ω : domain occupied by the material

Usual definition of w : derivative of Ψ_Ω w.r.t. u

$\rightarrow$ No longer valid

New definition : variational derivative of Ψ_Ω w.r.t. u

$\rightarrow w = -\alpha\Delta u + f(u)$

Energy decay (compatible boundary conditions) :

$$\frac{d\Psi_\Omega}{dt} = -\kappa \|\nabla w\|^2_{L^2(\Omega)^n} \leq 0$$

$$\frac{d\Psi_\Omega}{dt} = -\frac{1}{\kappa} \|\frac{\partial u}{\partial t}\|^2_{H^{-1}(\Omega)} \leq 0$$

Remark : If A and B are the two components : $u_A + u_B = 0$ (after rescaling) The Cahn-Hilliard equation is equivalent to a system of 2 Cahn-Hilliard equations

Free energy :

$$\Psi_\Omega(u_A, \nabla u_A, u_B, \nabla u_B) = \frac{1}{2}\int_\Omega (\frac{\alpha}{2}|\nabla u_A|^2 + \frac{\alpha}{2}|\nabla u_B|^2 + F(u_A) + F(u_B))dx$$

Equations :

$$\frac{\partial u_A}{\partial t} = \kappa\Delta(w_A - w_B),\ w_A = \frac{1}{2}(-\alpha\Delta u_A + f(u_A))\ (= \partial_{u_A}\Psi_\Omega)$$

$$\frac{\partial u_B}{\partial t} = \kappa\Delta(w_B - w_A),\ w_B = \frac{1}{2}(-\alpha\Delta u_B + f(u_B))\ (= \partial_{u_B}\Psi_\Omega)$$

$$u_A + u_B = 0,\ w_A + w_B = 0$$

$$w_A - w_B = -\alpha\Delta u_A + f(u_A)$$

Gradient term in the Ginzburg-Landau free energy : the interactions between the material's components are short-ranged

Obtained by approximation of a nonlocal term which also accounts for long-ranged interactions

Nonlocal Cahn-Hilliard equation : G. Giacomin-J.L. Lebowitz

Rigorous derivation based on stochastic arguments

Free energy :

$$\Psi_\Omega(u) = \int_{T^n} [f(u(x)) + u(x) \int_{T^n} \mathcal{K}(|x-y|)(1-u(y))dy]dx$$

T^n : n-dimensional torus, $\mathcal{K}$: smooth kernel

Mathematical analysis : C.G. Gal, H. Gajewski, M. Grasselli, ...

Usual boundary conditions :

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

$\Omega \subset R^N,\ N \leq 3$: bounded and regular domain
$\Gamma = \partial\Omega$
ν : unit outer normal vector

$\rightarrow$ 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

We can prove that

$$|u(t,x)| < 1 \text{ a.e } (t,x)$$

In one and two space dimensions :

$$\|u(t)\|_{L^\infty(\Omega)} \leq 1 - \delta,\ t > 0,\ \delta \in (0,1)$$

• 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

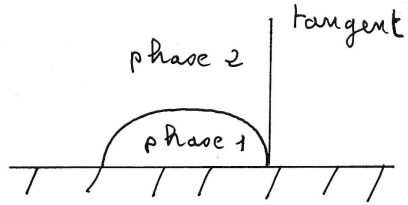
Mainly studied for polymer mixtures

Technological applications

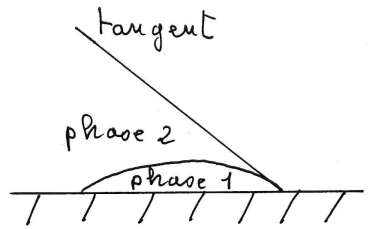
Problem : define the boundary conditions (we need 2 boundary conditions)

Variational boundary condition : static contact angle (not realistic)

$\theta > \frac{\pi}{2}$



$\theta = \frac{\pi}{2}$



$\theta < \frac{\pi}{2}$

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

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

the surface free energy

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

$\alpha_\Gamma > 0$
∇_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 : $\Psi = \Psi_\Omega + \Psi_\Gamma$

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

Energy decay :

$$\frac{d\Psi}{dt} = -\frac{1}{\kappa}\|\frac{\partial u}{\partial t}\|^2_{H^{-1}(\Omega)} - \frac{1}{d}\|\frac{\partial u}{\partial t}\|^2_{L^2(\Gamma)} \leq 0$$

Second 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

Cahn-Hilliard type equation on the boundary

Energy decay :

$$\frac{d\Psi_\Omega}{dt} = -\kappa \|\nabla \mu\|^2_{L^2(\Omega)^n} \leq 0$$

Third approach : C. Liu-H. Wu

Based on energetic principles

Similar boundary conditions + no mass flux at the boundary

Conservation of mass in the bulk and on the boundary separately

Regular potentials : the system is well understood

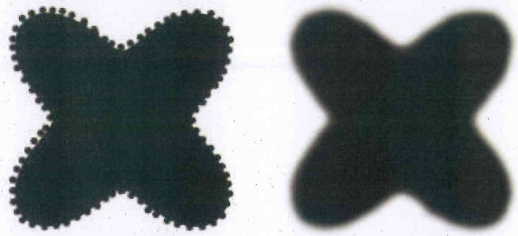
Contributors : R. Chill, C.G. Gal, E. Fašangová, A. Miranville, J. Pruess, R. Racke, H. Wu, S. Zelik, S. Zheng, ...

Singular potentials : more complicated and less understood

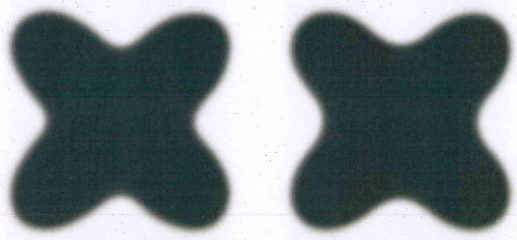
Possible nonexistence of classical solutions

Other applications of the Cahn-Hilliard equation :

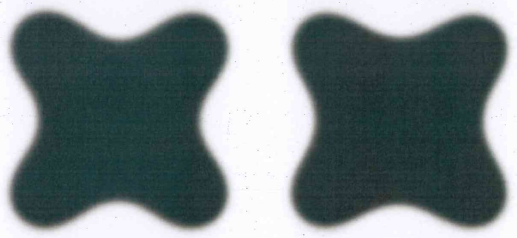
- Dealloying (corrosion processes)
- Population dynamics
- Bacterial films
- Thin films
- Image processing (denoising, inpainting)
- Astronomy (rings of Saturn)
- Clustering of mussels



(a) $t = 0$ (b) $t = 5 \cdot 10^{-8}$

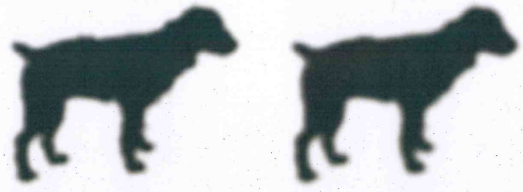


(c) $t = 5 \cdot 10^{-7}$ (d) $t = 5 \cdot 10^{-6}$

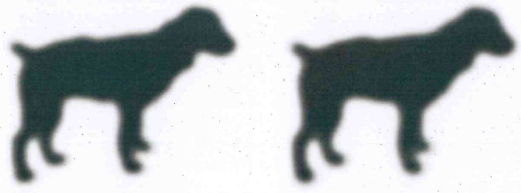


(e) $t = 2.5 \cdot 10^{-5}$ (f) $t = 5 \cdot 10^{-5}$

(a) $t = 0$ (b) $t = 2.5 \cdot 10^{-9}$



(c) $t = 5 \cdot 10^{-9}$ (d) $t = 10^{-8}$



(e) $t = 2.5 \cdot 10^{-8}$ (f) $t = 5 \cdot 10^{-8}$

A variant of the Cahn-Hilliard equation :

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

First model : The Cahn-Hilliard-Oono equation (Y. Oono-S. Puri, 1987)

$$g(x,s) = \beta s,\ \beta \geq 0$$

$\beta = 0$: Cahn-Hilliard equation

$\beta > 0$: models long-ranged (nonlocal) interactions

Introduced also to simplify numerical simulations

Associated free energy :

$$\Psi = \int_\Omega \left(\frac{\alpha}{2}|\nabla u|^2 + F(u) + \int_\Omega u(y)h(y,x)u(x)\,dx\right) dy$$

(Cahn-Hilliard equation : $\Psi = \int_\Omega \left(\frac{\alpha}{2}|\nabla u|^2 + F(u)\right) dx$)

h : models the long-ranged interactions ; Oono's model (N=3) :

$$h(y,x) = \frac{\beta}{4\pi|y-x|}$$

The long-ranged interactions are repulsive when $u(y)$ and $u(x)$ have the same sign

$\rightarrow$ Favors the formation of interfaces

Evolution equation :

$$\frac{\partial u}{\partial t} = \kappa \Delta \frac{\delta \Psi}{\delta u}$$

$\frac{\delta}{\delta u}$: variational derivative

$-\frac{1}{4\pi|y-x|}$: Green's function associated with the Laplace operator

Mathematical analysis : A. Miranville, JAAC ; A. Giorgini-M. Grasselli-A. Miranville, M3AS

Remarks :

a) Variant of the model (R. Choksi-X. Ren, 2003) :

$$g(x,s) = \beta(s - \frac{1}{\mathrm{Vol}(\Omega)} \int_\Omega u_0(x)\, dx)$$

u_0 : initial condition

Models microphase separation of diblock copolymers

Conservation of mass

Efficient numerical simulations (multigrid solvers) : A. Aristotelous-O. Karakashian-S. Wise

b) Coupling with the incompressible Navier-Stokes equations (Y. Huo-X. Jiang-H. Zhong-Y. Yang, 2003) :

Models a chemically reacting incompressible binary fluid in a bounded domain

Mathematical Analysis : S. Bosia-M. Grasselli-A. Miranville, M2AS

Second model : A Cahn-Hilliard/Allen Cahn equation (M. Hildebrant-A. Mikhailov, 1996)

System of equations :

$$\begin{aligned} \frac{\partial u}{\partial t} &= \epsilon^2 D\Delta w - w \\ w &= -\Delta u + \frac{f(u)}{\epsilon^2},\ D, \epsilon > 0 \end{aligned}$$

Equivalent formulation :

$$\frac{\partial u}{\partial t} + \epsilon^2 D\Delta^2 u - \Delta(Df(u) + u) + \frac{f(u)}{\epsilon^2} = 0$$

Models microscopic mechanisms such as surface diffusion and adsorption/desorption

Mathematical analysis : H. Israel

Third model : A Cahn-Hilliard model with a proliferation term (E. Khain-L. Sander, 2008)

$$g(x,s) = \beta s(s-1),\ \beta > 0$$

Models wound healing and tumor growth (1D) or clustering of malignant brain tumor cells (2D)

Deals with cells which move, proliferate and interact via diffusion and cell-cell adhesion

u : local density of cells
F : local free energy, $F(s) = \frac{1}{4}a(s-\frac{1}{2})^4 + \frac{1}{2}b(s-\frac{1}{2})^2,\ a > 0$
β : proliferation rate

Mathematical analysis : L. Cherfils-A. Miranville-S. Zelik, DCDS B

Fourth model : A Cahn-Hilliard model for binary image inpainting (A. Bertozzi-S. Esedoglu-A. Gillette, 2007)

$$g(x,s) = \lambda_0(s - h(x))\chi_{\Omega\setminus D}(x),\ \lambda_0 > 0,\ D \subset\subset \Omega$$

Equation :

$$\frac{\partial u}{\partial t} + \epsilon\Delta^2 u - \frac{1}{\epsilon}\Delta f(u) + g(x,u) = 0,\ \epsilon > 0$$

$h(x)$: given image ($h \in L^2(\Omega)$)
D : inpainting domain (damaged region)
$f(s) = 4s^3 - 6s^2 + 2s$
$g(x,u)$: added to keep u close to the image $h(x)$ outside the inpainting region (fidelity term)

Mathematical Analysis : L. Cherfils-H. Fakih-A. Miranville, IPI, SIIMS

Other variants of the Cahn-Hilliard equation :

Viscous Cahn-Hilliard equation

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

Proposed by A. Novick-Cohen to account for viscosity effects in the phase separation of polymer/polymer systems

Further generalizations : Microforce balance (M. Gurtin)

Take into account anisotropy, deformations of the material (e.g., elastic or visco-elastic materials), heat transfers

Hyperbolic Cahn-Hilliard equation

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

Proposed by P. Galenko et al. to model the early stages of spinodal decomposition in certain glasses

No mass conservation

Main difficulty : good notion of a solution in 2 and 3D

Bounded energy solutions : uniqueness in 2D

Logarithmic nonlinear terms : open problem ; already very difficult for the weakly damped wave equation :

$$\beta \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} - \Delta u + f(u) = 0,\ \beta > 0$$

Convective Cahn-Hilliard equation

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

Describes the dynamics of driven systems such as faceting of growing thermodynamically unstable crystal surfaces

Mass conservation

Cubic nonlinear term : A. Eden-V. Kalantarov

Logarithmic nonlinear terms : open problems (uniqueness, regularity)

Higher-order Cahn-Hilliard models

Free energy :

$$\Psi_{\mathrm{HOGL}} = \int_{\Omega} \left(\frac{1}{2} \sum_{i=1}^{M} \sum_{|k|=i} a_k |\mathcal{D}^k u|^2 + F(u)\right) dx, \; M \in N$$

$|k| = k_1 + k_2 + k_3, \; k = (k_1, k_2, k_3) \in (N \cup \{0\})^3$

$\mathcal{D}^k = \frac{\partial^{|k|}}{\partial x_1^{k_1} \partial x_2^{k_2} \partial x_3^{k_3}}$

Proposed by G. Caginalp-E. Esenturk to account for anisotropy effects

Corresponding equation :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i=1}^{M} (-1)^i \sum_{|k|=i} a_k \mathcal{D}^{2k} u - \Delta f(u) = 0$$

Examples :

Anisotropic Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} + \Delta \sum_{i=1}^{3} a_i \frac{\partial^2 u}{\partial x_i^2} - \Delta f(u) = 0$$

Sixth-order anisotropic Cahn-Hilliard equation :

$$\frac{\partial u}{\partial t} - \Delta \sum_{i,j=1}^{3} a_{ij} \frac{\partial^4 u}{\partial x_i^2 \partial x_j^2} + \Delta \sum_{i=1}^{3} b_i \frac{\partial^2 u}{\partial x_i^2} - \Delta f(u) = 0$$

Other sixth-order models :

- Strong anisotropy effects
- Atomistic models of crystal growth
- Description of growing crystalline surfaces with small slopes which undergo faceting
- Oil-water-surfactant mixtures
- Mixtures of polymer molecules

Regular nonlinear terms : well understood (L. Cherfils, M. Grasselli, A. Miranville, S. Peng, G. Schimperna, H. Wu, ...)

Logarithmic nonlinear terms : existence of classical solutions is open

Variational solutions : A. Miranville

Systems of Cahn-Hilliard equations

Multi-component materials

Stochastic Cahn-Hilliard equation

Also called Cahn-Hilliard-Cook equation

Takes into account thermal fluctuations

Coupling with the Allen-Cahn equation

Allen-Cahn equation :

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

Models the ordering of atoms during the phase separation

Coupling with the incompressible Navier-Stokes equations

Models mixtures of two incompressible immiscible fluids

$$\frac{\partial u}{\partial t} - \xi \mathrm{div} D(u) + (u \cdot \nabla)u + \nabla p = \varepsilon w \nabla \rho$$

$$\mathrm{div} u = 0$$

$$\frac{\partial \rho}{\partial t} + (u \cdot \nabla)\rho = \kappa \Delta w$$

$$w = -\varepsilon \Delta \rho + \frac{1}{\varepsilon} f(\rho)$$

$D(u) = \frac{1}{2}(\nabla u + {}^t\nabla u)$: deformation tensor
$\varepsilon w \nabla \rho$: Korteweg force

Boundary conditions : No slip boundary condition not realistic, dynamic boundary conditions

$$u \cdot \nu = 0, \ \frac{\partial \mu}{\partial \nu} = 0 \text{ on } \Gamma$$

$$\xi (D(u) \cdot \nu)_\Gamma + \beta u_\Gamma = \mathcal{L}(\rho) \nabla_\Gamma \rho \text{ on } \Gamma$$

$$\frac{\partial \rho}{\partial t} + u_\Gamma \cdot \nabla_\Gamma \rho = -l_0 \mathcal{L}(\rho) \text{ on } \Gamma$$

$$\mathcal{L}(\rho) = -\gamma \Delta_\Gamma \rho + \varepsilon \frac{\partial \rho}{\partial \nu} + \zeta \rho + g(\rho)$$

$l_0, \beta, \zeta \ \gamma > 0$: phenomenological parameters
β : slip coefficient
For $v : \Gamma \to \mathbb{R}^n$: $v_\nu = v \cdot \nu$ (normal component), $v_\Gamma = v - (v_\nu)\nu$ (tangential component)

Uniqueness : logarithmic nonlinear terms, dynamic boundary conditions (cubic and logarithmic nonlinear terms)

Variants : Cahn-Hilliard-Hele-Shaw, Cahn-Hilliard-Brinkman, Compressible Navier-Stokes equations