Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffusion systems, Phase fields Models. Application to Batteries and image processing **Part 1: Mathematical Setting**

Jean-Paul CHEHAB

LAMFA UMR CNRS 7352, Univ. Picardie Jules Verne

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Introduction



2 Basics of Elliptic and parabolic PDEs

Poisson problems and Boundary conditions

Plan

- Reaction-Equation
- Diffusion- Equation
- Reaction-diffusion equations

Introduction



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- Reaction-Equation
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Phase Fields

- Allen-Cahn model
- Allen-Cahn model : Gradient Flow and Minimization of an Energy

Plan

Cahn-Hilliard Equation

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- Cahn-Hilliard Equation

Allen-Cahn vs Cahn Hilliard

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Cahn-Hilliard Equation

Allen-Cahn vs Cahn Hilliard

- Annex
 - Stability of a differential system

Phase Fields Models : model natural phenomena

- material science : in complex fluids and soft matter
- Intercalation and conversion in batteries
- Biology, Medecine, Ecology : tumor growth, polluant transport in fluids
- Image processing : image segmentation, inpainting

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In Mathematics (a very actual and active topic)

- Mathematical analysis (dynamical systems, calculus of variations) [Temam88, Elliott89, Bertozzi, Miranville, Grasselli Pierre *et al*]
- Mathematical modeling
- Numerical analysis[Elliot89,Eyre94] and [Boyer, Shen,Wise,Pierre]

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Goal of the lecture

- Give simple basics of mathematical and numerical approach to phase fields
- Introduce to a friendly numerical environment that allows to produce nice numerical simulations (help in modeling)
- Special focus on Allen-Cahn and Cahn-Hilliard equations

Our approach to Allen-Cahn's model

Two approaches can be considered for studying Allen-Cahn's equation :

Reaction-Diffusion

$$\frac{\partial u}{\partial t} - \Delta u + \frac{1}{\epsilon^2} f(u) = 0$$
Reaction-diffusion approach

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• $\frac{\partial u}{\partial t} - \Delta u = 0$: parabolic equation

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Gradient Flow $\frac{\partial u}{\partial t} + \nabla E(u) = 0$ Gradient Flow approach

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• Use directly methods devoted to such structured equations

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• E(u) is time decreasing

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These two approaches coincide when $-\Delta u + \frac{1}{c^2}f(u) = \nabla E(u)$

Gradient Flow

$$\frac{\partial u}{\partial t} + \nabla E(u) = 0$$

Gradient Flow approach

- Use directly methods devoted to such structured equations
- E(u) is time decreasing

Notations

$\ln \mathbb{R}^n$

The gradient vector and laplacian of
$$F : \mathbb{R}^n \to \mathbb{R}$$
 at $x = (x_1, x_2, \cdots, x_n) \in \mathbb{R}^n$
 $\nabla F(x) = (\frac{\partial F(x)}{\partial x_1}, \cdots, \frac{\partial F(x)}{\partial x_n})^T$ and $\Delta F = \sum_{i=1}^n \frac{\partial^2 F(x)}{\partial x_i^2}$ Taylor $\in \mathbb{R}^n$:
 $F(x + ty) = F(x) + t < \nabla F(x), y > + \text{ lot }; < x, y > = \sum_{i=1}^n x_i y_i.$

In a functional space

Let Ω be an open and bounded set of \mathbb{R}^n . We define $\langle u, v \rangle = \int_{\Omega} uvdx$ If in a addition $\partial\Omega$, the boundary of Ω , is smooth enough, we can define the outise normal \vec{n} of Ω at $x \in \partial\Omega$ as the unit vector pointing outside Ω and orthogonal to the tangent plane at Ω in x. $\frac{\partial u}{\partial n} = \nabla u.\vec{n}$: normal derivative of u at x The Green formula : $\int_{\Omega} -\Delta uvdx = \int_{\Omega} \nabla u \nabla vdx - \int_{\partial\Omega} \frac{\partial u}{\partial n} ud\sigma = \int_{\Omega} u - \Delta vdx + \int_{\partial\Omega} \frac{\partial v}{\partial n} vd\sigma$

Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

Elliptic Equation

Let $\Omega \subset \mathbb{R}^n$, n = 1, 2, 3 for the applications, the spatial variables are $x_i, i = 1, \cdots, n$. We look to a function satisfying the PDE

$$\alpha u - \sum_{i,j=1}^{n} \frac{\partial}{\partial x_{i}} \left(a_{i,j} \frac{\partial}{\partial x_{j}} \right) = f \quad x \in \Omega,$$
(1)

+ Boundary Conditions on $\partial \Omega$

(2)

 $\partial \Omega$ is the boundary of Ω . The Boundary conditions are necessary to give a mathematical sense to this problem. They traduce a physical hypothesis.

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Canonical example

When
$$a_{i,j}(x) = \delta_{i,j} = \begin{cases} 1 & \text{if } i = j, \\ 0 & \text{else} \end{cases}$$
 the above equation reads :
 $\alpha u - \Delta u = f \quad x \in \Omega, \qquad (3)$
+ Boundary Conditions on $\partial \Omega$ (4)

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Basics of Elliptic and parabolic PDEs Phase Fields

Poisson problems and Boundary conditions

Dirichlet Problem

$$\alpha u - \Delta u = f \quad x \in \Omega,$$

$$u = g \quad \text{on } \partial\Omega \quad \text{Dirichlet Boundary conditions}$$
(6)

on $\partial \Omega$ Dirichlet Boundary conditions u = g

Here both f and g are given. The values of u are fixed on $\partial \Omega$. If g = 0: Homogeneous Dirichlet BC. This problem possesses a unique solution for every $\alpha \geq 0.$

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Poisson problems and Boundary conditions Reaction-Equation Diffusion-Equation



Figure - Isovalues of the Solution of a Poisson problem with Dirichlet BC)

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Neumann Problem

$$\alpha u - \Delta u = f \quad x \in \Omega, \tag{7}$$

 $\frac{\partial u}{\partial n} = g$ on $\partial \Omega$ Neumann Boundary conditions (8)

Here both f and g are given. The **fluxes** of u are **fixed** on $\partial\Omega$: $\frac{\partial u}{\partial n} = \nabla u \vec{n}$, where \vec{n} is the external normal vector. If g = 0: Homogeneous Neumann BC. This problem possesses a unique solution for every $\alpha > 0$.

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Poisson problems and Boundary conditions Reaction-Equation Diffusion-Equation Reaction diffusion equations



Figure – Isovalues of the Solution of a Poisson problem with Neumann BC

Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

Mixed Dirichlet-Neumann Problem

$-\Delta u = f$	$x\in\Omega,$		(9)
$\frac{\partial u}{\partial n} = g$	on $\partial\Omega_1$	Neumann Boundary Conditions	(10)
u = h	on $\partial\Omega_2$	Dirichlet Boundary Conditions	(11)

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Figure - Isovalues of the Solution of a Poisson problem with mixed BC

Poisson problems and Boundary conditions Reaction-Equation Reaction-diffusion equations

Consider the scalar ODE

$$\frac{du}{dt} = F(u) \tag{12}$$

$$u(0) = u_0$$
(Initial Condition) (13)

It is an ODE.

Properties

- Existence and uniqueness (under conditions on *F*) (without exsitence nothing can be done ... without unicity you don't know what your are computing...)
- Regularity (important for justifying approximation techniques)

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Poisson problems and Boundary conditions Reaction-Equation Reaction-diffusion equations

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Long time behaviour

- Steady state u^{*}/F(u^{*}) = 0
- Periodic solutions in time
- Chaos

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Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

Stablility of Steady states (see Annex for the higher dimensional case)

- u^* is stable if for every u(0) close enough to u^* , u(t) remains close to u^*
- u^* is asymptotically stable if for every u(0) close enough to u^* , $u(t) \rightarrow u^*$ as $t \rightarrow +\infty$
- u^* is **unstable** in the other cases
- Linear stability
 - Write the ODE near a steady state u^* : set $u(t) = u^* + \omega(t)$

$$f(u(t)) = f(u^* + \omega(t)) = \underbrace{f(u^*) + f'(u^*)\omega(t)}_{\text{by Taylor's formula}} + \operatorname{lower terms}_{\simeq f'(u^*)\omega(t)}$$

Since $\frac{du}{dt} = \frac{du^* + \omega(t)}{dt} = \frac{d\omega(t)}{dt}$, we can write the linearized ODE at u^* $\frac{d\omega(t)}{dt} = f'(u^*)\omega(t)$

whose solution is $\omega(t) = e^{f'(u^*)t}\omega(0)$.

• Hence u^* is stable if $f'(u^*) \le 0$ (asymptotically stable if $f'(u^*) < 0$), it is unstable otherwise.

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Logistic equation

Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

$$\frac{du}{dt} = \frac{1}{\epsilon^2} u(1 - u^2), \tag{14}$$

$$u(0) = u_0 \tag{15}$$

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Logistic equation

$$\frac{du}{dt} = \frac{1}{\epsilon^2} u(1 - u^2), \tag{14}$$

$$u(0) = u_0 \tag{15}$$

• Steady states are
$$u = 0$$
, $u = 1$ and $u = -1$

• Let
$$f(u) = \frac{1}{\epsilon^2}u(1-u^2)$$
. We have $f'(u) = \frac{1}{\epsilon^2}(1-3u^2)$

<i>u</i> *	$f'(u^*)$	Stability
0	$\frac{1}{\epsilon^2} > 0$	unstable
1	$-\frac{2}{\epsilon^2} < 0$	asymp. stable
-1	$-\frac{2}{\epsilon^{2}} < 0$	asymp. stable

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Figure – Evolution of the solution for different initial data for $\epsilon = 1$

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Figure – Evolution of the solution for different initial data for $\epsilon = 0.1$

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Poisson problems and Boundary condition Reaction-Equation Diffusion-Equation Reaction-diffusion equations



Figure – Evolution of the solution for different initial data for $\epsilon = 0.01$

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Poisson problems and Boundary conditions Reaction-Equation Reaction-diffusion equations

Consider now a functional ODE

$$\frac{du}{dt} = \frac{1}{\epsilon^2} u(1 - u^2), \tag{16}$$

$$u(x,0) = u_0(x)$$
 (17)

where u(x, 0) is now a given function of the variable $x \in [0, 1]$

(a)

Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

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where u(x, 0) is now a given function of the variable $x \in [0, 1]$ The solution of this equation can be expressed as

$$u(x,t) = \frac{u_0(x)}{\sqrt{u_0(x)^2 + (1 - u_0(x)^2) * e^{-2\frac{t}{e^2}}}}$$

We see that $u(x, t) \rightarrow sign(u_0(x))$ as $t \rightarrow +\infty$, so exactly what was observed in the scalar case.

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Figure – Solution at $t = 0 \epsilon = 1$ (random initial datum)

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Figure – Solution at $t = 2 \epsilon = 1$

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Figure – Solution at $t = 4 \epsilon = 1$

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Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations



Figure – Solution at $t = 6 \epsilon = 1$

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Figure – Solution at $t = 8 \epsilon = 1$

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The prototype is the Heat equation : it models the evolution of the distribution of heat in a domain, with given boundary condition and external source :

$$\frac{\partial u}{\partial t} - \Delta u = f \qquad \Omega, \tag{18}$$

(19)

+ Boundary Conditions on $\partial \Omega$, (20)

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Poisson problems and Boundary conditions Reaction-Equation Diffusion-Equation Reaction-diffusion equations

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Mathematical Properties

- Existence and Uniqueness
- Regularization
- When f is not time-dependent : when $t \to +\infty$, convergence to a steady state u^* solution of an elliptic equation

$$-\Delta u = f$$

with proper boundary conditions

• Stability (energy inequality)

Poisson problems and Boundary condition Reaction-Equation Diffusion-Equation Reaction-diffusion equations



Figure – Solution at t = 0 (brownian-type initial datum)

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Figure – Solution at t = 0.1

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Figure – Solution at t = 0.2

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Figure – Solution at t = 0.3

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Figure – Solution at t = 0.4

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Figure – Solution at t = 0.5

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Figure – Solution at t = 0.6

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Poisson problems and Boundary conditions Reaction-Equation Reaction-diffusion equations

We can write them into the form

$$\frac{\partial u}{\partial t} - \Delta u = F(u) \qquad \Omega, \tag{21}$$

(22) (23)

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+ Boundary Conditions on $\partial \Omega$,

Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

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(22)

(23)

 $+ \ {\rm Boundary} \ {\rm Conditions} \quad \ {\rm on} \ \partial\Omega,$

The source term F(u) (the reaction term) depends on u

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Poisson problems and Boundary conditions Reaction-Equation Diffusion- Equation Reaction-diffusion equations

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The source term F(u) (the reaction term) depends on u There is a competition between the two terms $-\Delta u$ and F(u). As in the nonlinear ODE case

Properties

- Existence and uniqueness (under conditions on *F*) (without existence nothing can be done ... without unicity you don't know what your are computing...)
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Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

By definition, a phase field model is a mathematical model for solving interfacial problems

Main characteristics

they model the dynamical minimization of a physical free energy. According to the conservation of mass property, we distinguish two type of equations

- Allen-Chan, gradient flow with no mass conservation; It models phase transition
- Cahn-Hilliard, which is mass conservative and models phase separation

Application domains

- material science : in complex fluids and soft matter (interfacial fluid flow, polymer science and in industrial applications).
- Intercalation and conversion in batteries
- Biological Science, Medecine and ecology : tumor growth, polluant transport in fluids
- Image processing : inpainting, image segmentation

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

Allen-Cahn equation is a and writes as

$$\frac{\partial u}{\partial t} + M(-\Delta u + \frac{1}{\epsilon^2}f(u)) = 0$$
(24)

$$\frac{\partial u}{\partial n} = 0 \tag{25}$$

$$u(0,x) = u_0(x)$$
 (26)

• It describes the process of phase separation in iron alloys [Allen-Cahn, 1972, 1973], including order-disorder transitions : M is the **mobilty** (taken to be 1 for simplicity), $F = \int_{-\infty}^{u} f(v) dv$ is the free energy, u is the

(non-conserved) order parameter, ϵ is the interface length.

- $\bullet\,$ The homogenous Neumann boundary condition implies that there is not a loss of mass outside the domain $\Omega\,$
- there is a competition between the potential term and the diffusion term : regularization in phase transition
- Maximum principle : if |u₀(x)| ≤ β then |u(x, t)| ≤ β, where β is the magnitude of largest zero of f.
- It is a reaction-diffusion equation !!

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Er Cahn-Hilliard Equation

Derivation

Minimize the Energy $E(u) = \frac{1}{2} \int_{\Omega} |\nabla u|^2 dx + \frac{1}{\epsilon} \int_{\Omega} F(u) dx$, where F is the potential of the free energy. The first term (Dirichlet energy) makes the phase transition smooth.

some potentials

- Double Well potential $F(u) = \frac{1}{4}(1-u^2)^2$ or Ginzburg-Landau double Well potential
- Truncated double-well potential

$$\tilde{F}(u) = \begin{cases} \frac{3M^2 - 1}{2}u^2 2M^3 u + \frac{1}{4}(3M^4 + 1) & \text{if } u > M\\ \frac{1}{4}(1 - u^2)^2 & \text{if } u \in [-M, M]\\ \frac{3M^2 - 1}{2}u^2 + 2M^3 u + \frac{1}{4}(3M^4 + 1) & \text{if } u < -M \end{cases}$$

Logarithmic free energy

$$F(u) = \frac{\theta}{2} (1+u) \ln 1 + u + (1-u) \ln 1 - u - \frac{\theta_c}{2} u^2$$

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

Gradient Flow basics :
$$\frac{du}{dt} = -\nabla E(u)$$

Definition and properties

• Energy decreasing : using the rule
$$\frac{dE(u)}{dt} = \langle \nabla E(u), \frac{du}{dt} \rangle$$
, we have

$$rac{dE(u)}{dt} = - <
abla E(u),
abla E(u) >= - \|
abla E(u)\|^2 \leq 0$$

- The steady state of the system are the critical points of E(u)
- When E is coercive $(E(u) \to +\infty \text{ as } ||u|| \to +\infty)$, the stable steady state are the minima of E(u)

Allen-Cahn as a Gradient flow

We let
$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\omega} F(u) dx$$

We have $\nabla E(u) = -\Delta u + \frac{1}{\epsilon^2} f(u)$ with f = F'. We recover Allen-Cahn's equation.

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Figure – Solution of AC : initial data (uniform randomly in [0,1])

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Figure – Solution of AC at time t =

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Figure – Solution of AC at time t =

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Figure – Solution of AC at time t =

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Figure - Allen Cahn : Initial datum

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Figure – Solution at t = after phase separation

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A first application in image processing : the image segmentation

$$\frac{\partial \phi}{\partial t} - \Delta \phi + \frac{F'(\phi)}{\epsilon^2} + \lambda \left((1+\phi)(f_0 - c_1)^2 - (1-\Phi)(f_0 - c_2)^2 \right), \quad x \in \Omega(27)$$
$$\frac{\partial \Phi}{\partial n} = 0, \qquad \partial \Omega \quad (28)$$

If C is the segmenting curve, then the phase ϕ corresponds to the situations

$$\phi(x) = \begin{cases} >0 & \text{if } x \text{ is inside } C, \\ =0 & \text{if } x \in C, \\ <0 & \text{if } x \text{ is outside } C, \end{cases}$$

Here $\epsilon > 0$, $F'(\phi) = \phi(\phi^2 - 1)$, λ is a nonnegative parameter, f_0 is the given image. The terms c_1 and c_2 are the averages of f_0 in the regions ($\phi \ge 0$) and ($\phi < 0$), say

$$c_1 = \frac{\int_\Omega f_0(x)(1+\phi(x))dx}{\int_\Omega (1+\phi(x))dx} \text{ and } c_2 = \frac{\int_\Omega f_0(x)(1-\phi(x))dx}{\int_\Omega (1-\phi(x))dx}$$

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Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

original image







Figure – Photograph. Segmentation $\Delta t = 5.e - 7$, $\epsilon = 0.04$, $\tau = 1$, $\lambda = 10^{10}$

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original image





segmented image

Figure – House. Segmentation $\Delta t = 5.e - 7$, $\epsilon = 0.04$, $\tau = 1$, $\lambda = 10^{10}$

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

The CH equation describes the process of phase separation, by which the two components of a binary fluid spontaneously separate and form domains pure in each component. It writes as

$$\frac{\partial u}{\partial t} - \Delta(-\Delta u + \frac{1}{\epsilon^2}f(u)) = 0, \qquad (29)$$

$$\frac{\partial u}{\partial n} = 0, \tag{30}$$

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$$\frac{\partial}{\partial n} \left(\Delta u - \frac{1}{\epsilon^2} f(u) \right) = 0, \tag{31}$$

$$u(0,x) = u_0(x)$$
 (32)

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

Derivation

Minimize the Energy E(u) with a conservation of the mass. Write the equation as a gradient flow :

$$\frac{\partial u}{\partial t} = \mathcal{L}(\frac{\partial}{\partial u}E(u))$$

Where \mathcal{L} is an operator such that $\int_{\Omega} \mathcal{L}(\frac{\partial}{\partial u} \mathcal{E}(u)) dx = 0$. A simple choice is $\mathcal{L} = D\nabla .[\phi(u)\nabla(.)]$, where D is the diffusion and ϕ is the mobility, eg, when $\phi = 1$, $\mathcal{L} = D\Delta$.

Properties

- Conservation of the mass : $\bar{u} = \int_{\Omega} u(x,t) dx = \int_{\Omega} u_0(x) dx$
- Decay of the energy in time

$$\frac{\partial E(u)}{\partial t} = -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \le 0$$

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CH as coupled system

A nice way to study and to simulate CH is to decouple the equation as follows :

$$\frac{\partial u}{\partial t} - \Delta \mu = 0, \tag{33}$$

$$\mu = -\Delta u + \frac{1}{\epsilon^2} f(u), \tag{34}$$

$$\frac{\partial u}{\partial n} = 0, \tag{35}$$

$$\frac{\partial \mu}{\partial n} = 0, \tag{36}$$

$$u(0,x) = u_0(x)$$
 (37)

Application domains

material science : in complex fluids and soft matter (interfacial fluid flow, polymer science and in industrial applications).

Biological Science and Medicine : tumor growth

Image processing : inpainting (see also hereafter)

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Time Simulations

- 2D phase separation https://www.youtube.com/watch?v=52ZDH9mzDtc • Link
- 3D phase separation (in a cube) https://www.youtube.com/watch?v=ROd6EMoLdjQ → Link (in a sphere) https://www.youtube.com/watch?v=CrGatXppcrc → Link
- mussels pattern https://www.youtube.com/watch?v=u-mEjfBaYks
 Link

4 2 5 4 2 5
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Pattern dynamics, corsening



Eiguro - Cobp Hilliord concorring : t-0 - 0.01 (At - 0.01) Jean-Paul CHEHAB Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Pattern dynamics, corsening



Figure – Cabe Hilliard coarcening : +=0.001 c = 0.001 (A + = 0.001) Jean-Paul CHEHAB Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Pattern dynamics, corsening



Eiguro - Cabe Hilliard coarconing : t=0.002 c= 0.001 (A+=0.001) Jean-Paul CHEHAB Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Pattern dynamics, corsening



Eiguro - Cabe Hilliard coarconing : t=0.003 c=0.001 (A+=0.001) Jean-Paul CHEHAB Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Eiguro - Cabn Hilliard coarroning : + -0.01 - -0.001 (A+ -0.001) Jean-Paul CHEHAB Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Pattern dynamics, corsening



Eiguro – Cabn Hilliard coarconing : + – 0.02 – – 0.001 (A+ – 0.001) Jean-Paul CHEHAB Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Pattern dynamics, corsening

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Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

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Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

A first application in image processing : the inpainting

The inpainting is the process of reconstructing lost or deteriorated parts of images (photos as well as videos) : the idea is to take off the detoriated part (mask) and to recover in this region the rest of the original image. This can be done by using several techniques, one of them being based on Cahn-Hilliard equations. • Link

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Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

A Cahn-Hilliard mathematical model for the inpainting

Let g be the original image and $D \subset \Omega$ the region of Ω in which the image is deterred. The idea is to add a penalty term that forces the image to remain unchanged in $\Omega \setminus D$ and to reconnect the fields of g inside D. Let $\lambda >> 1$

$$\frac{\partial u}{\partial t} - \Delta(-\epsilon\Delta u + \frac{1}{\epsilon}f(u)) + \lambda\chi_{\Omega\setminus D}(x)(u-g) = 0,$$
(38)

Cahn-Hilliard equation

Fidelity term (39)

$$\frac{\partial u}{\partial n} = 0 \quad \frac{\partial}{\partial n} \left(\Delta u - \frac{1}{\epsilon^2} f(u) \right) = 0, \tag{40}$$

$$u(0,x) = u_0(x)$$
 (41)

Here $\chi_{\Omega \setminus D}(x) = \begin{cases} 1 & \text{if } x \in \Omega \setminus D, \\ 0 & \text{else} \end{cases}$

- The presence of the penalization term $\lambda \chi_{\Omega \setminus D}(x)(u-g)$ forces the solution to be close to g in $\Omega \setminus D$ when $\lambda >> 1$
- The Cahn-Hilliard flow has as effect to connect the fields inside D
- here
 e will play the role of the "contrast". A post-processing is possible
 using a thresholding procedure.

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Illustration with a simple example : the inpainting of a triangle.



Figure – Inpainting with-C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, N = 128 – Initial inpainted image left (t = 0) right (t = 0.05) = 2 Jan-Paul (HEHAB) Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

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Figure – Inpainting with-C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, N = 128 – Initial inpainted image left (t = 0) right (t = 0.01) (HEHAB 2) = 100000 Continuum Modeling: Numerical schemes for linear & nonlinear reaction/diffu

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Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

Illustration with a 3D example : the inpainting of a box



Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

Illustration with a 3D example : the inpainting of a box



Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

Illustration with a 3D example : the inpainting of a box



Figure – Inpainting with-C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, N = 128 – Initial inpainted image left (t = 0) right (t = 0.05) (t = 0.05) (t = 0.0000) (t = 0.0000)

Allen-Cahn model Allen-Cahn model : Gradient Flow and Minimization of an Energy Cahn-Hilliard Equation

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Figure – Inpainting with-C-H. $\Delta t = 0.001$, $\epsilon = 0.05$, N = 128 – Initial inpainted image left (t = 0) right (t = 0.05) (HEHAB 2) = 100000 Jaan-Paul (HEHAB 2) = 100000

Allen-Cahn

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

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Allen-Cahn

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

Allen-Cahn

$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\Omega} F(u) dx$$

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Allen-Cahn

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$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\Omega} F(u) dx$$

u is **not** conserved

$$\frac{du}{dt} = -\nabla E(u)$$

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Allen-Cahn

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$$\frac{du}{dt} = -\nabla E(u)$$

Double Well Potential

$$F(u) = \frac{1}{\epsilon^2} \frac{1}{4} (1 - u^2)^2$$
$$f(u) = F'(u)$$

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Cahn-Hilliard

$$\frac{\partial E(u)}{\partial t} = -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \le 0$$

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Allen-Cahn

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

Allen-Cahn

$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\Omega} F(u) dx$$

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Double Well Potential

$$F(u) = \frac{1}{\epsilon^2} \frac{1}{4} (1 - u^2)^2$$
$$f(u) = F'(u)$$

Cahn-Hilliard

$$\frac{\partial E(u)}{\partial t} = -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \le 0$$

u is locally conserved, according to Fick's second law $\frac{du}{dt}=-\nabla J$

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Allen-Cahn

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

Allen-Cahn

$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\Omega} F(u) dx$$

u is **not** conserved

$$\frac{du}{dt} = -\nabla E(u)$$

Double Well Potential

$$F(u) = \frac{1}{\epsilon^2} \frac{1}{4} (1 - u^2)^2$$
$$f(u) = F'(u)$$

Cahn-Hilliard

$$\frac{\partial E(u)}{\partial t} = -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \le 0$$

u is locally conserved, according to
Fick's second law $\frac{du}{dt} = -\nabla J$
Define the potential
 $\mu = -\Delta u + F'(u)$

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Allen-Cahn

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

Allen-Cahn

$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\Omega} F(u) dx$$

u is not conserved

$$\frac{du}{dt} = -\nabla E(u)$$

Double Well Potential

$$F(u) = \frac{1}{\epsilon^2} \frac{1}{4} (1 - u^2)^2$$
$$f(u) = F'(u)$$

Cahn-Hilliard

$$\frac{\partial E(u)}{\partial t} = -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \le 0$$

u is locally conserved, according to Fick's second law $\frac{du}{dt} = -\nabla J$ Define the potential $\mu = -\Delta u + F'(u)$ Constitutive equation

$$J = -M(u)\nabla\mu$$

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Allen-Cahn

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

Allen-Cahn

$$E(u) = \frac{1}{2} \int_{\Omega} \|\nabla u\|^2 dx + \frac{1}{\epsilon^2} \int_{\Omega} F(u) dx$$

u is **not** conserved

$$\frac{du}{dt} = -\nabla E(u)$$

Double Well Potential

$$F(u) = \frac{1}{\epsilon^2} \frac{1}{4} (1 - u^2)^2$$
$$f(u) = F'(u)$$

Cahn-Hilliard

$$\begin{split} \frac{\partial E(u)}{\partial t} &= -\int_{\Omega} |\nabla(-\Delta u + \frac{1}{\epsilon^2}f(u))|^2 dx \leq 0\\ u \text{ is locally conserved, according to}\\ \text{Fick's second law } \frac{du}{dt} &= -\nabla J\\ \text{Define the potential}\\ \mu &= -\Delta u + F'(u)\\ \text{Constitutive equation}\\ J &= -M(u)\nabla\mu\\ f(u) &= F'(u) \end{split}$$

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In higher dimension we consider the differential system :

$$\frac{du}{dt} = F(u) \tag{42}$$

$$u(0) = u_0 \in {\rm I\!R}^n$$
 (Initial Condition) (43)

Her $F : \mathbb{R}^n \to \mathbb{R}^n$ is a regular function. We will assume that properties of existence and uniqueness of the solution as well as those of regularity are satisfied. We just here extend the analysis of stability of the steady states of the differential system.

The linear case

Consider the case F(u) = Au - b. When A is invertible, the only steady state is the solution of the linear system $Au^* = b$. We can write any vector $v \in \mathbb{R}^n$ as $v = u^* + w$. Then

$$\frac{dw}{dt} = Aw$$

We have formally w(t) = exp(tA)w(0). Then w(t) remains bounded iff the eigenvalues of A are of negative real part. If their real part is strictly negative, w(t) converges to 0 as $t \to +\infty$: this is the asymptotic stability.

Linear stability in dimension n

Let u^* be a steady state, i.e. $F(u^*)=0$. As in the scalar case, we write the system near u^* : set $u(t)=u^*+\omega(t)$

$$egin{aligned} & F(u(t)) & = F(u^*) + JF(u^*)\omega(t) + ext{lower terms} \end{aligned}$$

by Taylor's formula

 $\simeq JF'(u^*)\omega(t)$

Here $JF(u^*)$ is the jacobian matrix of F at u^* , say $(JF(u^*))_{i,j} = \frac{\partial F_i(u^*)}{\partial x_i}$.

- If none of the eigenvalues of $JF(u^*)$ is pure imaginary, then the local stability is similar to the one in the linear case
- We cannot conclude with the spectral argument if there is at least a couple of pure imaginary eigenvalues.

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