

Bsc Thesis

Jonathan Ulmer

November 22, 2023

Contents

1	Cahn Hillard Equation Overview	1
1.1	TODO Derivation from paper	2
1.1.1	Free energy	2
1.1.2	Derivation by mass balance	2
2	Baseline Multigrid solver:	3
2.1	Discretization: ATTACH	3
2.2	adaptations to the simplified problem	4
2.3	tests _{data} :	4
2.3.1	squares	4
2.3.2	circles	7
2.4	Tests	7
3	Relaxed Problem	7
3.1	TODO relaxed operators:	7
3.1.1	L Relaxed	7
3.1.2	SMOOTH	7
4	References	8

1 Cahn Hillard Equation Overview

Partial Differential Equation (PDE) solving the state of a 2 Phase Fluid[2].
The form of the Cahn Hillard Equation used for the remainder of this thesis
is:

$$\phi_t(x, t) = \Delta \mu \tag{1}$$

$$\mu = -\varepsilon^2 \Delta \Phi + W'(\Phi) \tag{2}$$

where ϕ is the so called phase field. Demarking the different states of the fluids through an Interval $I = [-1, 1]$ and where $\partial I = \{-1, 1\}$ represents full state of one fluid. $\varepsilon > 0$ is a positive constant

, and μ is the chemical potential[2]. While the Cahn Hillard exist in a more general form taking the fluids mobility $M(\Phi)$ into account, we will assume $M(\Phi) = 1$, simplifying the CH-Equations used in[2][1] to what is stated above.

The Advantages of the Cahn Hillard Approach as compared to traditional fluid dynamics solvers are for example: “explicit tracking of the interface” [2], as well as “evolution of complex geometries and topological changes [...] in a natural way” [2]

1.1 TODO Derivation from paper

1.1.1 Free energy

The Cahn Hillard Equations can be motivated Using a **Ginzburg Landau** type free energy equation:

$$E^{\text{bulk}} = \int_{\Omega} \frac{\varepsilon^2}{2} |\nabla \phi|^2 + F(\phi) dx$$

where “ $F(\phi)$ denotes the (Helmholtz) free energy density of mixing.” [2] and will be approximated in further calculations as $F(\phi) = \frac{(1-\phi^2)^2}{4}$ as used in[1]

The chemical potential then follows as derivative of Energy in respect to time.

$$\mu = \frac{\delta E_{\text{bulk}}(\phi)}{\delta \phi} = -\varepsilon^2 \Delta \phi + W'(\phi)$$

1.1.2 Derivation by mass balance

The Cahn Hillard equation then can be motivated as follows: consider

$$\partial_t \phi + \nabla \cdot \mathbf{J} = 0 \tag{3}$$

where \mathbf{J} is mass flux. eq1 then states that the change in mass balances the change of the phasefield. using the no-flux boundary conditions:

$$\mathbf{J} \cdot \mathbf{n} = 0 \quad \partial \Omega \times (0, T) \tag{4}$$

$$\partial_n \phi = 0 \quad \partial \Omega \times (0, T) \tag{5}$$

conservation of mass follows see[2].

using:

$$J = -\nabla\mu \quad (6)$$

which conceptionally sets mass flux to equalize the the potential energy gradient, leads to the formulation of the CH equations as stated above. additionally the boundry conditions evaluate to:

$$\begin{aligned} -\nabla\mu &= 0 \\ \partial_n\phi &= 0 \end{aligned}$$

ie no flow leaves and potential on the border doesn't change. then for ϕ then follows:

$$\begin{aligned} \frac{d}{dt}E^{bulk}(\phi(t)) &= \int_{\Omega} (\varepsilon^2 \nabla\phi \cdot \nabla\partial_t\phi + W'(\phi)\partial_t\phi) dx \\ &= - \int_{\Omega} |\nabla\mu|^2 dx, \end{aligned} \quad \forall t \in (0, T)$$

hence the Free Energy is decreasing in time.

2 Baseline Multigrid solver:

As baseline for further experiments a multi grid method based on finite differences by[1]. is used.

2.1 Discretization:

ATTACH

it discretizes the phasefield and potential energy ϕ, μ into a grid wise functions ϕ_{ij}, μ_{ij} and defines the partial derivatives $D_x f_{ij}, D_y f_{ij}$ using the differential quotients:

$$D_x f_{i+\frac{1}{2}j} = \frac{f_{i+1j} - f_{ij}}{h} \quad D_y f_{ij+\frac{1}{2}} = \frac{f_{ij+1} - f_{ij}}{h}$$

for $\nabla f, \Delta f$ then follows:

$$\begin{aligned} \nabla f_{ij} &= (D_x f_{i+1j}, D_y f_{ij+1}) \\ \Delta f_{ij} &= \frac{D_x f_{i+\frac{1}{2}j} - D_x f_{i-\frac{1}{2}j} + D_y f_{ij+\frac{1}{2}} - D_y f_{ij-\frac{1}{2}}}{h} = \nabla_d \cdot \nabla_d f_{ij} \end{aligned}$$

the authors further adapt the discretized phasefield by the characteristic function of the domain Ω :

$$G(x, y) = \begin{cases} 1 & (x, y) \in \Omega \\ 0 & (x, y) \notin \Omega \end{cases}$$

To account for boundry conditions and arbitrary shaped domains. The authors [1] then define the discrete CH Equation adapted for Domain, as:

$$\begin{aligned} \frac{\phi_{i+1j} - \phi_{ij}}{\Delta t} &= \nabla_d \cdot (G_{ij} \nabla_d \mu_{ij}^{n+1}) \\ \mu_{ij}^{n+1} &= 2\phi_{ij}^{n+1} - \varepsilon^2 \nabla_d \cdot (G_{ij} \nabla_d \phi_{ij}^{n+1}) + W'(\phi_{ij}^n) - 2\phi_{ij}^n \end{aligned}$$

and derive the iteration operator $L(\phi^{n+1}, \mu^{n+\frac{1}{2}}) = (\zeta^n, \psi^n)$

$$L \begin{pmatrix} \phi^{n+1} \\ \mu^{n+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \frac{\phi^{n+1}}{\Delta t} - \nabla_d \cdot (G_{ij} \nabla_d \mu^{n+\frac{1}{2}}) \\ \varepsilon^2 \nabla_d \cdot (G_{ij} \nabla_d \phi_{ij}^{n+1}) - 2\phi_{ij}^{n+1} + \mu_{ij}^{n+\frac{1}{2}} \end{pmatrix}$$

initialized as $(\zeta^n, \psi^n) = \begin{pmatrix} \frac{\phi_{ij}^{n+1}}{\Delta t} \\ W'(\phi_{ij}^n) - 2\phi_{ij}^n \end{pmatrix}$ the algorithm is then defined as:

wherein SMOOTH consists of point-wise Gauß Seidel Relaxation , by solving L for $\bar{\phi}, \bar{\mu}$ with the initial guess for ζ^n, ψ^n .

2.2 adaptations to the simplified problem

even tough this work uses rectangular domains, the adaptation of the algorithm is simplified by the domain indicator function, as well as 0 padding, in order to correctly include the boundry conditions of the CH equation. therefore the internal representation of the adapted algorithm considers phasefield and potential field ϕ, μ as 2D arrays of shape $(N_x + 2, N_y + 2)$ in order to accommodate padding. Where N_x and N_y are the number of steps in x- / y-Direction respectively. Hence, we define the discrete domain function as:

$$G_{ij} = \begin{cases} 1 & (i, j) \in [1, N_x + 1] \times [1, N_y + 1] \\ 0 & \text{else} \end{cases}$$

2.3 tests_{data}:

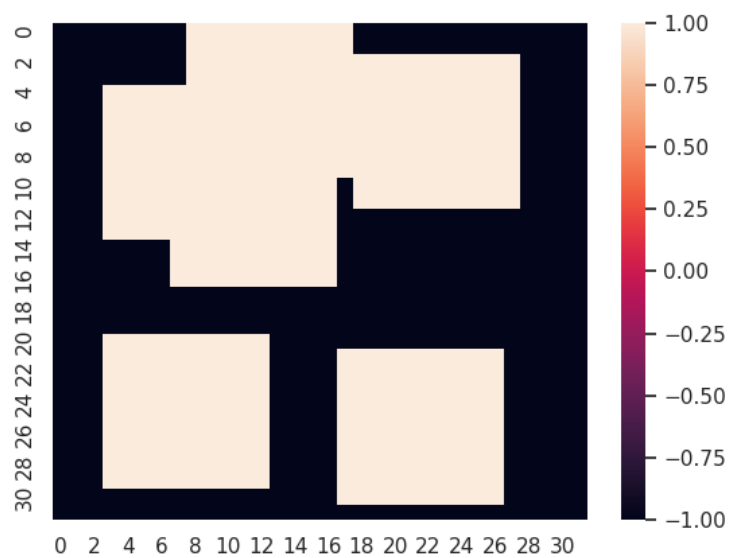
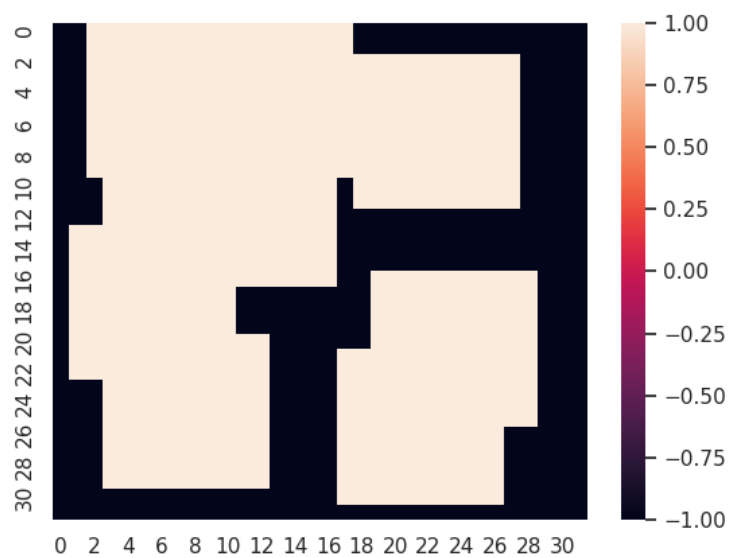
2.3.1 squares

For testting and later training , a multitude o different phasefields where used. notably an assortment of rrandomly lpaced circles, squares, and arbertrary generated values



/home/proceduraltree/org/.attach/20/5127bc-bc81-41a2-b5e4-509fc6a555b7/_20231031_12

Figure 1: FAS Multigrid v-cycle as defined by [1]



2.3.2 circles

2.4 Tests

3 Relaxed Problem

In effort to decrease the order of complexity, the following relaxation to the classical CH Equation is proposed:

3.1 TODO relaxed operators:

3.1.1 L Relaxed

$$L \begin{pmatrix} \phi^{n+1} \\ \mu^{n+1} \end{pmatrix} = \begin{pmatrix} \frac{\phi_{ij}^{n+1,m}}{\Delta t} - \nabla_d \cdot (G_{ji} \nabla_d \mu_{ji}^{n+\frac{1}{2},m}) \\ \varepsilon^2 (c^\alpha - (\phi_{ij}^{n+1,m})^\alpha) - 2\phi_{ij}^{n+1,m} - \mu_{ji}^{n+\frac{1}{2},m} \end{pmatrix}$$

3.1.2 SMOOTH

$$SMOOTH(\phi_{ij}^{n+1,m}, \mu_{ji}^{n+\frac{1}{2},m}, L_h, \zeta^n, \psi^n)$$

$$\begin{aligned} \bar{\mu}_{ji}^{n+\frac{1}{2},m} &= \frac{\phi_{ij}^{n+1,m}}{\Delta t} - \zeta_{ij}^n \\ &\quad - \frac{1}{h^2} (G_{i+\frac{1}{2}j} \mu_{i+1j}^{n+\frac{1}{2},m} + G_{i-1j} \mu_{i-1j}^{n+\frac{1}{2},m} + G_{ij+1} \mu_{ij+1}^{n+\frac{1}{2},m} + G_{ij-1} \mu_{ij-1}^{n+\frac{1}{2},m}) \\ &\quad \cdot (G_{i+1j} + G_{i-1j} + G_{ij+1} + G_{ij-1})^{-1} \\ \varepsilon^2 (\bar{\phi}_{ij}^{n+1,m})^\alpha + 2\phi_{ij}^{n+1,m} &= \varepsilon^2 c^\alpha - \mu_{ji}^{n+\frac{1}{2},m} - \psi_{ij} \end{aligned}$$

1. Proposal design newton method to solve second equation (in conjunction with the first one) hopefully solving is faster than the original multiple SMOOTH Iterations. The iteration is to solve for $\phi_{ij}^{n+1,m}$ as free variable. Therefore it follows for $F(x)$

$$\begin{aligned} F(x) &= \varepsilon^2 x^\alpha + 2x - \varepsilon^2 c^\alpha + y + \psi_{ij} \\ y &= \frac{x}{\Delta t} - \zeta_{ij}^n \\ &\quad - \frac{1}{h^2} (G_{i+\frac{1}{2}j} \mu_{i+1j}^{n+\frac{1}{2},m} + G_{i-1j} \mu_{i-1j}^{n+\frac{1}{2},m} + G_{ij+1} \mu_{ij+1}^{n+\frac{1}{2},m} + G_{ij-1} \mu_{ij-1}^{n+\frac{1}{2},m}) \\ &\quad \cdot (G_{i+1j} + G_{i-1j} + G_{ij+1} + G_{ij-1})^{-1} \end{aligned}$$

And the derivative for the iteration is

$$\begin{aligned}\frac{d}{dx}F(x) &= \alpha\varepsilon^2x^{\alpha-1} + 2 + \frac{d}{dx}y \\ \frac{d}{dx}y &= \frac{1}{\Delta t}\end{aligned}$$

4 References

References

- [1] Jaemin Shin, Darae Jeong, and Junseok Kim. “A conservative numerical method for the Cahn–Hilliard equation in complex domains”. In: *Journal of Computational Physics* 230.19 (2011), pp. 7441–7455. ISSN: 0021-9991. DOI: <https://doi.org/10.1016/j.jcp.2011.06.009>. URL: <https://www.sciencedirect.com/science/article/pii/S0021999111003585>.
- [2] Hao Wu. “A review on the Cahn–Hilliard equation: classical results and recent advances in dynamic boundary conditions”. In: *Electronic Research Archive* 30.8 (2022), pp. 2788–2832. DOI: [10.3934/era.2022143](https://doi.org/10.3934/era.2022143). URL: <https://doi.org/10.3934/era.2022143>.