Bsc Thesis

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Contents

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.

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

1.1.2 Derivation by mass balance

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

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

where **J** is mass flux. eq1 then states that the change in mass balances the change of the phasefield. using the no-flux boundry conditions:

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

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

conservation of mass follows see[2].

using:

$$J = -\nabla \mu \tag{6}$$

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:

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

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:

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

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 $\overline{\phi}, \overline{\mu}$ 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 $\mathrm{N_x}$ and $\mathrm{N_y}$ 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$_{\mathbf{data}}$:

2.3.1 squares

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

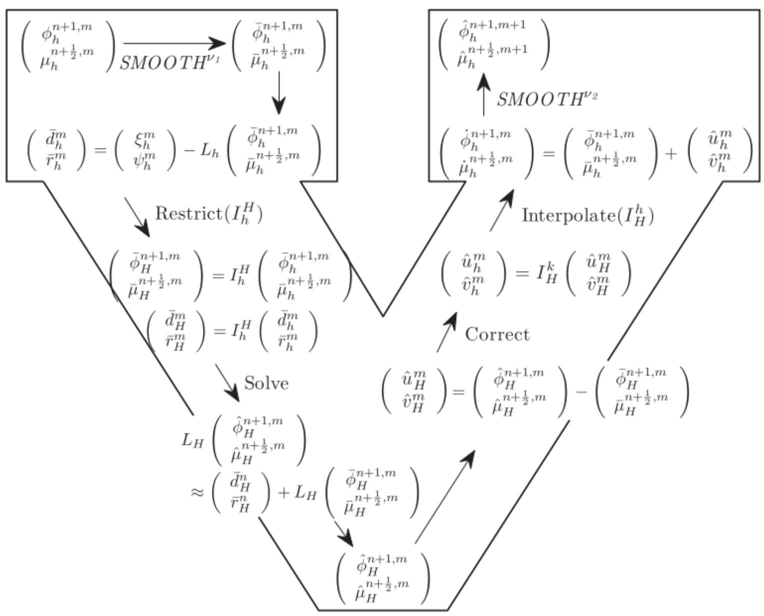
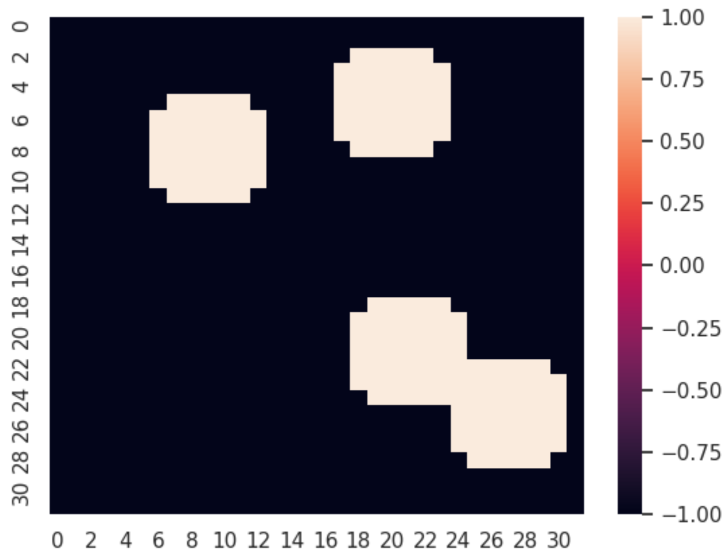
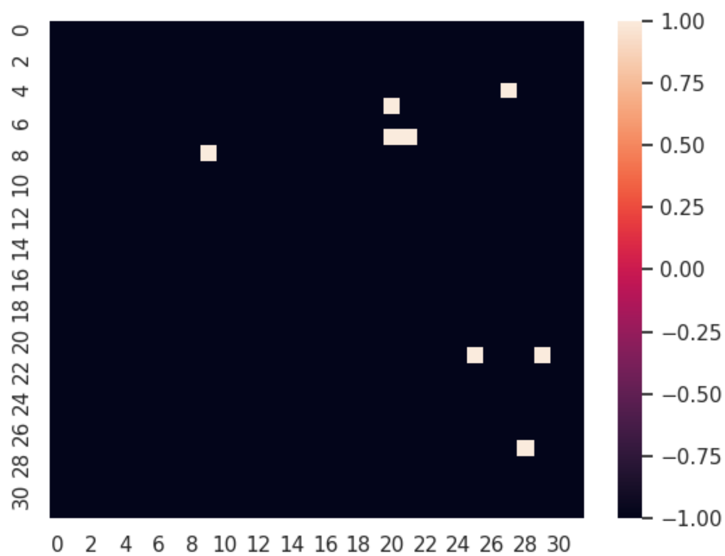


Figure 1: FAS Multigrid v-cycle as defined by [1]


0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00


0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30
0 2 4 6 8 10 12 14 16 18 20 22 24 26 28 30
1.00
0.75
0.50
0.25
0.00
−0.25
−0.50
−0.75
−1.00

2.3.2 circles

2.4 Tests

```
test_phase = tu.random_phase()
solver = tu.setup_solver(test_phase)
solver.solve(4,10)
plt.figure()
sns.heatmap(solver.phase_small)
```

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

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

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

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

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

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`. URL: `https://doi.org/10.3934%2Fera.2022143`.