Bsc Thesis

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Contents

1 Cahn Hillard Equation Overview

Partial Differential Equation (PDE) solving the state of a 2 Phase Fluid[**Wu_2022**]. 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[**Wu_2022**]. 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[**Wu_2022**][**SHIN20117441**] 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" [**Wu_2022**], as well as "evolution of complex geometries and topological changes [. . .] in a natural way" [**Wu_2022**]

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."" [**Wu_2022**] and will be approximated in further calculations as $F(\phi) = \frac{(1-\phi^2)^2}{4}$ as used in[**SHIN20117441**]

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:

$$J \cdot n = 0 \qquad\qquad \partial\Omega \times (0, T) \qquad\qquad (4)$$
$$\partial_n \phi = 0 \qquad\qquad \partial\Omega \times (0, T) \qquad\qquad (5)$$

conservation of mass follows see[**Wu_2022**].

using:

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

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:

$$-\nabla\mu = 0$$
$$\partial_n \phi = 0$$

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

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

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[**SHIN20117441**]. 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:

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

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

$$\nabla_d f_{ij} = (D_x f_{i+1j}, \ D_y f_{ij+1})$$
$$\Delta_d f_{ij} = \frac{D_x f_{i+\frac{1}{2}j} - D_x f_{i-\frac{1}{2}j} + D_y f_{ij+\frac{1}{2}} - D_y f_{ij-\frac{1}{2}}}{h} = \nabla_d \cdot \nabla_d f_{ij}$$

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 [**SHIN20117441**] then define the discrete CH Equation adapted for Domain, as:

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

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 N_x and N_y are the number of steps in x- / y-Direction respectively. Hence, we define the discrete domain function as:
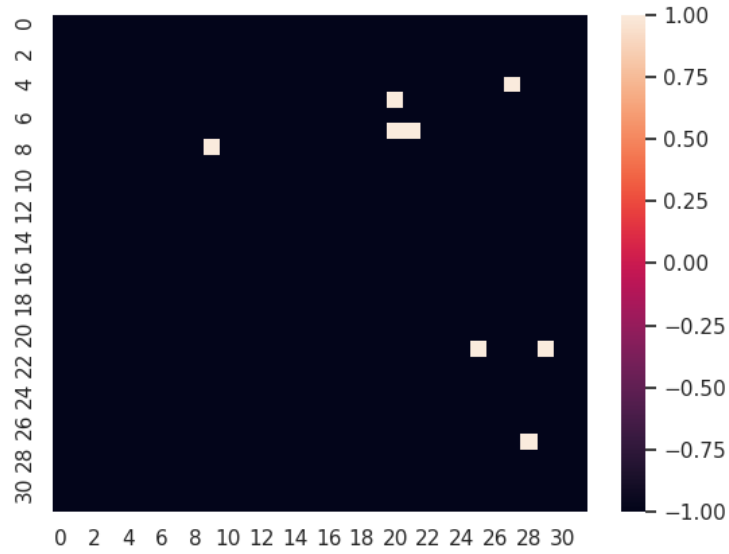
$$G_{ij} = \begin{cases} 1 & (i,j) \in [1, N_x + 1] \times [1, N_y + 1] \\ 0 & \text{else} \end{cases}$$

2.3   tests$_{\text{data}}$:

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
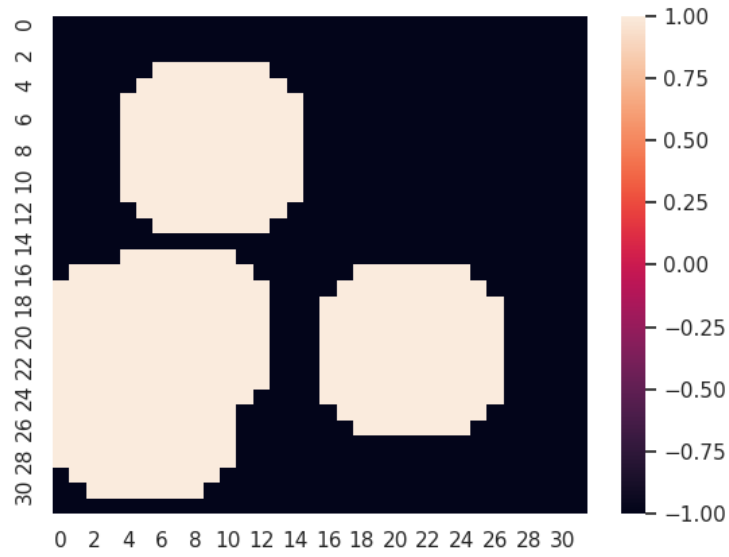
2.4 Tests

```
1  test_phase = tu.k_spheres_phase(4,7)
2  solver = tu.setup_solver(test_phase)
3  solver.solve(4,10)
```

```
1  plt.figure()
2  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

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

$$\bar{\mu}_{ji}^{n+\frac{1}{2},m}=\frac{\phi_{ij}^{n+1,m}}{\Delta t}-\zeta_{ij}^n$$
$$-\frac{1}{h^2}(G_{i+\frac{1}{2}j}\mu_{i+1j}^{n+\frac{1}{2},m}+G_{i-1j}\mu_{i-1j}^{n+\frac{1}{2},m}+G_{ij+1}\mu_{ij+1}^{n+\frac{1}{2},m}+G_{ij-1}\mu_{ij-1}^{n+\frac{1}{2},m})$$
$$\cdot(G_{i+1j}+G_{i-1j}+G_{ij+1}+G_{ij-1})^{-1}$$

$$\varepsilon^2(\bar{\phi}_{ij}^{n+1,m})^\alpha+2\phi_{ij}^{n+1,m}=\varepsilon^2c^\alpha-\mu_{ji}^{n+\frac{1}{2},m}-\psi_{ij}$$

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 $F(x)$

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

And the derivative for the iteration is

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

3.2   Elliptical PDE:

on order to solve the relaxed CH Equation the following PDE as to be solved in Each additional time step:

$$-\Delta c^\alpha + \alpha c^a = \alpha \phi^\alpha$$

or in terms of the characteristic function:

$$-\nabla \cdot (G\nabla c^\alpha) + \alpha c^\alpha = \alpha \phi^\alpha$$

3.2.1   Discretisation

$$-\nabla_d \cdot (G_{ij}\nabla c_{ij}^\alpha) + \alpha c_{ij}^\alpha = \alpha \phi_{ij}^\alpha$$

$$-(\frac{1}{h}(G_{i+\frac{1}{2}j}\nabla c_{i+\frac{1}{2}j}^\alpha + G_{ij+\frac{1}{2}}\nabla c_{ij+\frac{1}{2}}^\alpha)) = \alpha \phi_{ij}^\alpha$$

4   References