Bachelor Thesis

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Contents

This thesis follows reproducible research philosophy, in that we provide all relevant code in the same file as the writing itself. We then use this file to generate exports to html and PDF, as well as extract the code to be used independently. Further details on execution and reading of the original source provided in org-mode format is provided in 7

1 The Cahn-Hilliard equation

The Cahn-Hilliard(CH) equation is a partial differential equation (PDE) solving the state of a two-phase fluid[**Wu_2022**]. The form of the CH equation used in this thesis is

$$\begin{aligned} \partial_t \phi(x,t) &= \nabla \cdot (M(\phi)\nabla\mu) \\ \mu &= -\varepsilon^2 \Delta\phi + W'(\phi) \end{aligned} \tag{1}$$

where, ϕ is a phase-field variable representing the different states of the fluids through an interval $I = [-1, 1]$

$$\phi = \begin{cases} 1 & \phi = \text{phase 1} \\ -1 & \phi = \text{ phase 2} \end{cases}$$

ε is a positive constant correlated with boundary thickness and μ is the chemical potential[**Wu_2022**].

In this thesis we assume $M(\phi) \equiv 1$, simplifying the CH equation used in [**Wu_2022**] [**SHIN20117441**].

The advantages of the CH approach, as compared to traditional boundary coupling, 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**]. In practice it enables linear interpolation between different formulas on different phases.

1.1 Derivation from paper

1.1.1 The free energy

The authors in [**Wu_2022**] motivate the CH equation using the **Ginzburg-Landau** free energy equation:

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

where $W(\phi)$ denotes the (Helmholtz) free energy density of mixing[**Wu_2022**] that we approximate it in further calculations with $W(\phi) = \frac{(1-\phi^2)^2}{4}$ as in [**SHIN20117441**]. Additionally $\nabla \phi$ represents the change in phase-field.

The chemical potential, μ, then follows as the variational derivation of the free energy**??**.

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

1.1.2 Derivation by mass balance

The paper[**Wu_2022**] motivates us to derive the CH equation as follows:

$$\partial_t \phi + \nabla \cdot J = 0 \tag{2}$$

where J is mass flux. The equation 2 then ensures continuity of mass Using the no-flux boundary conditions:

$$J \cdot n = 0 \qquad \partial\Omega \times (0,T) \tag{3}$$

$$\partial_n \phi = 0 \qquad \partial\Omega \times (0,T) \tag{4}$$

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

$$\begin{aligned} \frac{d}{dt}\int_\Omega \phi &= \int_\Omega \frac{\partial \phi}{\partial t} dV \\ &= -\int_\Omega \nabla \cdot J \; dV \\ &= \int_{\partial\Omega} J \cdot n \; dA \\ &= 0 \end{aligned} \tag{5}$$

Therefore mass is conserved over time, as shown in 5. We define the mass flux, J, as the gradient in chemical potential as follows

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

This results in the CH equation as stated in 1.

$$\begin{aligned} -\nabla \mu &= 0 \\ \partial_n \phi &= 0 \end{aligned} \tag{7}$$

i.e. no flow leaves and potential on the border doesn't change. In order to show the CH equation's consistency with thermodynamics we take the time derivation of the free energy **??** and we show that it decreases in time.

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

2 Baseline multi-grid solver

As baseline for numerical experiments we use a two-grid method based on the finite difference method defined in[**SHIN20117441**].

2.1 The discretization of the CH equation:

It discretizes the phase-field ,ϕ, and chemical potential ,μ, into grid-wise functions ϕ_{ij}, μ_{ij} and defines the partial derivatives $D_x f_{ij},\ D_y f_{ij}$ using the differential quotients:

$$D_x f_{i+\frac{1}{2}j} = \frac{f_{i+1j} - f_{ij}}{h} \qquad D_y f_{ij+\frac{1}{2}} = \frac{f_{ij+1} - f_{ij}}{h} \tag{8}$$

For $\nabla f, \nabla \cdot \nabla f$ then follows:

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

The authors in [**SHIN20117441**] further adapt the discretized phase-field by the characteristic function of the domain Ω in order to satisfy the boundary conditions:

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

To simplify the notation for discretized derivatives we use the following abbreviations:

Math	Code
$\Sigma_G f_{ij} = G_{i+\frac{1}{2}j} f_{i+1j}^{n+\frac{1}{2},m} + G_{i-\frac{1}{2}j} f_{i-1j}^{n+\frac{1}{2},m} + G_{ij+\frac{1}{2}} f_{ij+1}^{n+\frac{1}{2},m} + G_{ij-\frac{1}{2}} f_{ij-1}^{n+\frac{1}{2},m}$	`discrete_weigted_neigbou`
$\Sigma_G = G_{i+\frac{1}{2}j} + G_{i-\frac{1}{2}j} + G_{ij+\frac{1}{2}} + G_{ij-\frac{1}{2}}$	`neighbours_in_domain(i,j`

We can then write the modified Laplacian $\nabla_d(G\nabla_d f_{ij})$ as:

$$\nabla_d \cdot (G\nabla_d f_{ij}) = \frac{\Sigma_G f_{ij} - \Sigma_G \cdot f_{ij}}{h^2}$$

We use this modified Laplacian to deal with boundary conditions. Our abbreviations simplify separating implicit and explicit terms in the discretization. The authors in [**SHIN20117441**] then define the discrete CH equation adapted for the domain as:

$$\begin{aligned} \frac{\phi_{ij}^{n+1} - \phi_{ij}^{n}}{\Delta t} &= \nabla_d \cdot (G_{ij} \nabla_d \mu_{ij}^{n+\frac{1}{2}}) \\ \mu_{ij}^{n+\frac{1}{2}} &= 2\phi_{ij}^{n+1} - \varepsilon^2 \nabla_d \cdot (G_{ij} \nabla_d \phi_{ij}^{n+1}) + W'(\phi_{ij}^{n}) - 2\phi_{ij}^{n} \end{aligned} \tag{9}$$

and derive a numerical scheme from this implicit equation.

2.2 Simplifications

The authors in[**SHIN20117441**] modelled the phase-field problem for complex shaped domains. Even tough this work uses rectangular domains, we simplify the adaptation of the algorithm by the domain indicator function, as well as 0 padding, in order to correctly include the boundary conditions of the CH equation. Therefore, the internal representation of the adapted algorithm considers phase-field ,ϕ, and chemical potential field ,μ, as two-dimensional arrays with the 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 implement the discrete domain function as:

$$G_{ij} = \begin{cases} 1, & (i,j) \in [2, N_x + 1] \times [2, N_y + 1] \\ 0, & \text{else} \end{cases}$$

2.3 PDE as operator L

We derive the iteration operator $L(\phi^{n+1}, \mu^{n+\frac{1}{2}}) = (\zeta^n, \psi^n)$as in[**SHIN20117441**].

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

This operator follows from 9 by separating implicit and explicit terms L and $(\zeta_{ij}^n, \psi_{ij}^n)^T$, respectively.

$$\begin{pmatrix} \zeta^n \\ \psi^n \end{pmatrix} = \begin{pmatrix} \frac{\phi_{ij}^n}{\Delta t} \\ W'(\phi_{ij}^n) - 2\phi_{ij}^n \end{pmatrix}$$

Due to being explicit, we know everything needed to calculate $(\zeta_{ij}^n, \psi_{ij}^n)^T$ at the beginning of each time step. We compute those values once and store them in the solver.

Furthermore, as it enables a Newton iteration, we derive its Jacobian with respect to the current grid point $(\phi_{ij}^{n+1}, \mu_{ij}^{n+\frac{1}{2}})^T$:

$$DL \begin{pmatrix} \phi \\ \mu \end{pmatrix} = \begin{pmatrix} \frac{1}{\Delta t} & \frac{1}{h^2}\Sigma_G \\ -\frac{\varepsilon^2}{h^2}\Sigma_G - 2 & 1 \end{pmatrix}$$

2.4 V-cycle approach

The numerical method proposed in [**SHIN20117441**] consists of a V-cycle multi-grid method derived from previously stated operators. Specificly we use a two-grid implementation consisting of

1. a Gauß-Seidel relaxation for smoothing.
2. restriction and prolongation methods between grids $h \leftrightarrow H$.
3. a Newton iteration to solve $L(x,y)_H = L(\bar{x}, \bar{y}) + (d_h, r_h)$.

The V-cycle of a two-grid method using pre and post smoothing is then stated by: So let's take a closer look at the internals, namely the phase field after pre-SMOOTHing $\bar{\phi}$, the phase residuals of $\left[L(\bar{\phi_{ij}}, \bar{\mu_{ij}}) - (\zeta_{ij}, \psi_{ij})\right]_{ij\in\Omega}$ and the result of the Newton iteration on coarsest level.

[width=.9]images/v$_cycle$

After a few iterations, V-cycle exhibits the following behavior:

`images/iteration.gif`

2.5 SMOOTH operator

The authors[**SHIN20117441**]derived Gauss-Seidel Smoothing from:

$$L \begin{pmatrix} \phi_{ij}^{n+1} \\ \mu_{ij}^{n+\frac{1}{2}} \end{pmatrix} = \begin{pmatrix} \zeta_{ij}^n \\ \psi_{ij}^n \end{pmatrix}$$

solved for ϕ, μ. 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.

$$SMOOTH(\phi_{ij}^{n+1,m}, \mu_{ji}^{n+\frac{1}{2},m}, L_h, \zeta^n, \psi^n) \tag{10}$$

and we implement it as

[width=.9]images/smooth

2.6 Test data:

For testing and later training we use a multitude of different phase-fields, notably an assortment of randomly placed circles, squares, and arbitrary generated values.

Size	blobs	blobsize	norm
64	10	10	2
64	10	10	100
512	20	50	2

[width=.9]testdata

Figure 1: Examples of different phase-fields used as the initial condition in this work.

3 Numerical evaluation

The analytical CH equation conserves mass 2 and the free energy ,E_{bulk}, **??** decreases in time, i.e. consistence with the second law of thermodynamics. Therefore, we use discrete variants of those concepts as necessary conditions for a "good" solution. Furthermore, since E_{bulk} is closely correlated with chemical potential, μ, we evaluate this difference as quality of convergence.

3.1 Energy evaluations

As discrete energy measure we use:

$$\begin{aligned} E^{\text{bulk}} &= \sum_{i,j\in\Omega} \frac{\varepsilon^2}{2}|G\nabla\phi_{ij}|^2 + W\left(\phi_{ij}\right)\, dx \\ &= \sum_{i,j\in\Omega} \frac{\varepsilon^2}{2}G_{i+\frac{1}{2}j}(D_x\phi_{i+\frac{1}{2}j})^2 + G_{ij+\frac{1}{2}}(D_y\phi_{ij+\frac{1}{2}})^2 + W\left(\phi_{ij}\right)\, dx \end{aligned}$$

#TODO Plot

3.2 Mass balance

Instead of a physical mass we use the average of ϕ over the domain Ω written as:

$$\frac{1}{|\Omega|}\int_{\Omega}\phi\ dx \tag{11}$$

We calculate this balance as:

$$b = \frac{\sum_{i,j\in\Omega}\phi_{ij}}{|\{(i,j)\in\Omega\}|}$$

such that $b = 1$ means there is only phase 1, $\phi \equiv 1$, and $b = -1$ means there is only phase 2, $\phi \equiv -1$.

3.3 Tests

`images/behaviour.gif`

3.4 rate of convergence

4 Relaxed problem

In effort to decrease the order of complexity, from fourth order derivative to second order, we propose an elliptical relaxation approach, where the relaxation variable c is the solution of the following elliptical PDE:

$$-\Delta c^{\alpha} + \alpha c^{a} = \alpha\phi^{\alpha},$$

where α is a relaxation parameter. We expect to approach the original solution of the CH equation 1 as $\alpha \to \infty$. This results in the following relaxation for the classical CH equation 1:

$$\begin{aligned}\partial_t\phi^{\alpha} &= \Delta\mu \\ \mu &= \varepsilon^2\alpha(c^{\alpha}-\phi^{\alpha}) + W'(\phi)\end{aligned} \tag{12}$$

It in turn requires solving the elliptical PDE each time-step to calculate c. We obtain a simpler approach in the numerical solver, with the drawback of having more variables. However those are independent. As ansatz for the numerical solver we propose:

$$\begin{aligned}\frac{\phi_{ij}^{n+1,\alpha}-\phi_{ij}^{n,\alpha}}{\Delta t} &= \nabla_d\cdot(G_{ij}\nabla_d\mu_{ij}^{n+\frac{1}{2},\alpha}) \\ \mu_{ij}^{n+\frac{1}{2},\alpha} &= 2\phi_{ij}^{n+1,\alpha} - \varepsilon^2 a(c_{ij}^{n+1,\alpha}-\phi_{ij}^{n+1,\alpha}) + W'(\phi_{ij}^{n,\alpha}) - 2\phi_{ij}^{n,\alpha}\end{aligned} \tag{13}$$

This approach is inspired by 13 adapted to the relaxed CH equation 9.

4.1 relaxed operators:

We then adapt the multi-grid solver proposed in 2 to the relaxed problem by replacing the differential operators by their discrete counterparts as defined in **??**, and expand them.

4.2 Relaxed PDE as operator L

We reformulate of the iteration in terms of Operator L as follows:

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

and its derivative:

$$DL\begin{pmatrix}\phi\\ \mu\end{pmatrix} = \begin{pmatrix}\frac{1}{\Delta t} & \frac{1}{h^2}\Sigma_G\\ -\varepsilon^2\alpha - 2 & 1\end{pmatrix}$$

4.3 SMOOTH operator

Correspondingly the SMOOTH operation expands to:

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

$$\begin{aligned} -\frac{\Sigma_G}{h^2}\overline{\mu_{ji}^{n+\frac{1}{2},m,\alpha}} &= \frac{\phi_{ij}^{n+1,m,\alpha}}{\Delta t} - \zeta_{ij}^{n,\alpha} - \frac{\Sigma_G \mu_{ij}}{h^2} \\ \varepsilon^2\alpha\overline{\phi_{ij}^{n+1,m,\alpha}} + 2\phi_{ij}^{n+1,m,\alpha} &= \varepsilon^2\alpha c_{ij}^{n,\alpha} - \overline{\mu_{ji}^{n+\frac{1}{2},m,\alpha}} - \psi_{ij}^{n,\alpha} \end{aligned} \tag{14}$$

We then solve directly for the smoothed variables, $\overline{\mu_{ij}^{n+1,m,\alpha}}$ and $\overline{\phi_{ij}^{n+1,m,\alpha}}$. This was not done in the original paper[**SHIN20117441**] because the required system of linear equations in the paper[**SHIN20117441**] was solved numerically. We simplify the relaxed system in one-dimension, and solve explicitly:

$$\varepsilon^2\alpha(\phi^\alpha) + 2\phi^\alpha = \varepsilon^2\alpha c^\alpha - \frac{h^2}{\Sigma_G}(\frac{\phi^\alpha}{\Delta t} - \zeta_{ij}^n - \frac{1}{h^2}\Sigma_G\mu_{ij}) - \psi_{ij}$$

$\implies$

$$\varepsilon^2\alpha(\phi^\alpha) + 2\phi^\alpha + \frac{h^2}{\Sigma_G}\frac{\phi^\alpha}{\Delta t} = \varepsilon^2\alpha c^\alpha - \frac{h^2}{\Sigma_G}(-\zeta_{ij}^n - \frac{1}{h^2}\Sigma_G\mu_{ij}) - \psi_{ij}$$

$\Longrightarrow$

$$(\varepsilon^2\alpha + 2 + \frac{h^2}{\Sigma_G \Delta t})\phi^\alpha = \varepsilon^2 \alpha c^\alpha - \frac{h^2}{\Sigma_G}(-\zeta_{ij}^n - \frac{\Sigma_G \mu_{ij}}{h^2}) - \psi_{ij}$$

$\Longrightarrow$

$$\phi^\alpha = \left(\varepsilon^2 \alpha c^\alpha - \frac{h^2}{\Sigma_G}(-\zeta_{ij}^n - \frac{\Sigma_G \mu_{ij}}{h^2}) - \psi_{ij}\right)\left(\varepsilon^2\alpha + 2 + \frac{h^2}{\Sigma_G \Delta t}\right)^{-1}$$

4.4 Relaxed V-cycle approach

As the difference between both methods is abstracted away in the operators, the relaxed V-cycle is identical to the original counterpart and therefore reused. The only additional step is solving the elliptical equation:

`images/iteration_relaxed2.gif`

4.5 Elliptical PDE:

In order to solve the relaxed CH equation we solve the following PDE in each time step:

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

Similarly to the first solver we solve this PDE with a finite difference scheme using the same discretization as before.

4.5.1 Discretization

The discretization of the PDE expands the differential operators in the same way and proposes an equivalent scheme for solving the elliptical equation **??**.

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

$\Longrightarrow$

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

$\Longrightarrow$

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

As before we abbreviate $\Sigma_G c^{\alpha}_{ij} = G_{i+\frac{1}{2}j} c^{\alpha}_{i+1j} + G_{i-\frac{1}{2}j} c^{\alpha}_{i-1j} + G_{ij+\frac{1}{2}} c^{\alpha}_{ij+1} + G_{ij-\frac{1}{2}} c^{\alpha}_{ij-1}$ and $\Sigma_G = G_{i+\frac{1}{2}j} + G_{i-\frac{1}{2}j} + G_{ij+\frac{1}{2}} + G_{ij-\frac{1}{2}}$. Then the discrete elliptical PDE can be stated as:

$$-\frac{\Sigma_G c^{\alpha}_{ij}}{h^2} + \frac{\Sigma_G}{h^2} c^{\alpha}_{ij} + \alpha c^{\alpha}_{ij} = \alpha \phi^{\alpha}_{ij} \tag{15}$$

1. **DONE** Proposal1 Newton Solver And then we propose a simple newton Iteration to solve 15 for $x = c^{\alpha}_{ij}$: Let F, dF be:

   $$F(x) = -\frac{\Sigma_G c^{\alpha}_{ij}}{h^2} + \frac{\Sigma_G}{h^2} x + \alpha x - \alpha \phi^{\alpha}_{ij}$$

   and $dF(x)$

   $$dF(x) = -\frac{\Sigma_G}{h^2} + \alpha$$

   the implementation then is the following:

   as input, we use :

2. Proposal2 solver solving 15 for c^{α}_{ij} then results in.

   $$\left(\frac{\Sigma_G}{h^2} + \alpha\right) c^{\alpha}_{ij} = \alpha \phi^{\alpha}_{ij} + \frac{\Sigma_G c^{\alpha}_{ij}}{h^2}$$

   and can be translated to code as follows

5 Comparison

`images/comparison.gif`

$$||\phi^{n+1}_{ij} - \phi^{n+1,\alpha}_{ij}|| \to 0 \tag{16}$$

In practice we observe the following behaviour:

[width=.9]images/alpha-error

6 AI

We propose a data motivated alternative to the elliptical PDE in the relaxed CH equation 13. We propose there to be a better solution then the discrete result of **??**. We define "better" as minimizing:

$$||\phi^{n+1} + \frac{1}{\alpha}\nabla \cdot (G\nabla\phi^{n+1}) - c||_{Fr} \tag{17}$$

in the Frobenious norm $||\cdot||_{Fr}$

7 Technical details

We are writing this thesis in org-mode file format.

8 References