

# Project Thesis

## Solving Cahn Hilliard Equation

Isak Hammer

March 23, 2022



# 1 Introduction

Introduction

## 2 Cahn Hilliard Equation on a Closed Membrane

Let  $c_0$  and  $c_1$  indicate the concentration profile of the substances in a 2-phase system such that  $c_0(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$  and similarly  $c_1(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$ , where  $\mathbf{x}$  is a element of some surface  $\Omega$  and  $t$  is time. However, in the 2 phase problem we will restrict ourself so that  $c_0(t, \mathbf{x}) + c_1(t, \mathbf{x}) = 1$  at any  $\mathbf{x}$  at time  $t$ . A property of the restriction is that we now can express  $c_0$  using  $c_1$ , with no loss of information. Hence, let us now define  $c = c_0$  so  $c(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$ . It has been shown that 2 phase system if thermodynamically unstabl can be evolve into a phase separation described by a evolutionary differential equation [1] using a model based on chemical energy of the substances. However, further development has been done [2] to solve this equation on surfaces. Now assume model that we want to describe is a phase-seperation on a closed membrane surface  $\Gamma$ , so that  $c(\mathbf{x}, t) : \Gamma \times [0, T] \rightarrow [0, 1]$ . Then is the surface Cahn Hilliard equation described such that

$$\rho \frac{\partial c}{\partial t} - \nabla_\Gamma (M \nabla_\Gamma (f'_0 - \varepsilon^2 \nabla_\Gamma^2 c)) = 0 \quad \text{on } \Gamma. \quad (1)$$

We define here the tangential gradient operator to be  $\nabla_\Gamma c = \nabla c - (\mathbf{n} \cdot \nabla c) \mathbf{n}$  applied on the surface  $\Gamma$  restricted to  $\mathbf{n} \cdot \nabla_\Gamma c = 0$ .

Lets define  $\varepsilon$  to be the size of the layer between the substances  $c_1$  and  $c_2$ . The density  $\rho$  is simply defined such that  $\rho = \frac{m}{S_\Gamma}$  is a constant based on the total mass divided by the total surface area of  $\Gamma$ . Here is the mobility  $M$  often derived such that is is dependent on  $c$  and is crucial for the result during a possible coarsening event [2]. However, the free energy per unit surface  $f_0 = f_0(c)$  is derived based on the thermodynamical model and should according to [2] be nonconvex and nonlinear.

A important observation is that equation (1) is a fourth order equation which makes it more challenging to solve using conventional FEM methods. This clear when writing the equation on the equivalent weak form and second order equations arise.

### 3 Hybrid Symmetric Interior Penalty DG Method on Heat Equation

Lets define the problem

$$\begin{aligned} -\varepsilon \nabla u &= f \quad \text{in } \Omega \\ u &= u_D \quad \text{on } \Gamma_D \\ \partial_n u &= g \quad \text{on } \Gamma_N \\ \partial_n u + \beta u &= h \quad \text{on } \Gamma_R \end{aligned}$$

Here is  $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$ . We want to write this on a weak form. Let the spaces we work on be

$$H^1(\mathcal{T}_h) = \{u \in L^2(\Omega), u \in H^1(T) \forall T \in \mathcal{T}_h\}$$

For the problem to be discontinuous do we define the trial and test function to be  $u \in H^1(\Omega)$  and  $v \in H^1(\mathcal{T}_h)$ . Thus,

$$-\sum_{T \in \mathcal{T}_h} \int_T \varepsilon \nabla^2 u \cdot v dx = \sum_{T \in \mathcal{T}_h} \left\{ \int_T \varepsilon \nabla u \nabla v dx - \int_{\partial T} \varepsilon \cdot \partial_n u \cdot v ds \right\} = \sum_{T \in \mathcal{T}_h} \int_T f \cdot v dx. \quad (2)$$

But we want to introduce the shorter notation equivalently such that

$$\sum_{T \in \mathcal{T}_h} \{ \varepsilon \langle \nabla u, \nabla v \rangle_T - \varepsilon \langle \partial_n u, v \rangle_{\partial T} \} = \sum_{T \in \mathcal{T}_h} (f, v). \quad (3)$$

Where  $\langle \cdot, \cdot \rangle$  is the surface integral operator. Before we continue do we want to introduce a alternative method to integrate using edges. Let  $v_F \in L^2(\mathcal{F}_h)$  for the set of all facets  $\mathcal{F}_h$ . Now the surface integral can be rewritten such that

$$\sum_{T \in \mathcal{T}_h} \varepsilon \langle \partial_n u, v_F \rangle = \sum_{E \in \mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E + \sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle. \quad (4)$$

Lets define some crucial spaces for the DG method

$$\begin{aligned} V &= \{(u, u_F) : u \in H^2(\mathcal{T}_h) \cap H^1(\Omega), u_F \in L^2(\mathcal{F}_h)\} \\ V_h &= \{(u, u_F) : u \in \mathcal{P}^k(T) \forall T \in \mathcal{T}_h, u_F \in \mathcal{P}^k(E) \forall E \in \mathcal{F}_h\} \end{aligned}$$

What is the intuition of a polynomial  $\mathcal{P}^k(E)$  along a edge?

and now including drichlet conditions using the previous definition

$$\begin{aligned} V_D &= \{(u, u_F) \in V, u_F = u_D \quad \text{on } \Gamma_D\} \quad V_{h,D} = \{(u, u_F) \in V_h, u_F = u_D \quad \text{on } \Gamma_D\} \\ V_0 &= \{(u, u_F) \in V, u_F = 0 \quad \text{on } \Gamma_D\} \quad V_{h,0} = \{(u, u_F) \in V_h, u_F = 0 \quad \text{on } \Gamma_D\} \end{aligned}$$

Defining  $(u, u_F) \in V_D$  and  $(v, v_F) \in V_0$ . Now adding (3) and (4) can we easily see that

$$\sum_{T \in \mathcal{T}_h} \{ \varepsilon \langle \nabla u, \nabla v \rangle_T \} = \sum_{T \in \mathcal{T}_h} (f, v) + \sum_{E \in \mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E + \sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle. \quad (5)$$

Applying the Neumann conditions on  $\Gamma_N$  and  $\Gamma_R$ , can the condition on the exterior facets be rewritten such that

$$\sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle = \varepsilon \langle g, v_F \rangle_{\Gamma_N} + \varepsilon \langle h - \beta u, v_F \rangle_{\Gamma_R}$$

Keep in mind that we on the exterior boundaries define the integral so  $\langle f, v_F \rangle = \int_{\Gamma} f \cdot v_F \cdot n ds$  for a arbitrary neumann boundary  $f$  on some surface  $\Gamma$ . Hence (5) ends up being

$$\sum_{T \in \mathcal{T}_h} \varepsilon \langle \nabla u, \nabla v \rangle - \sum_{E \in \mathcal{F}^{int}} (\varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E) + \langle \beta u, v_F \rangle_{\Gamma_R} = \sum_{T \in \mathcal{T}_h} (f, v) + \langle g, v_F \rangle_{\Gamma_N} + \langle h, v_F \rangle_{\Gamma_R}. \quad (6)$$

According to Lehrenfeld 2010 [3] at page 13 on equation (1.2.7) is (6) equivalent to

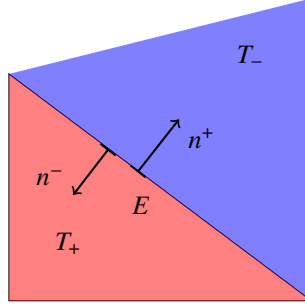


Figure 1: Edge  $E$  shared by the triangles  $T_-$  and  $T_+$  and the normal unit vectors  $n^+$  and  $n^-$ .

$$\sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} = \sum_{T \in \mathcal{T}_h} (f, v) + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \quad (7)$$

Where,  $u, u_F \in V_D$  and  $v, v_F \in V_h$ . Here is the jump defined simply as  $[v] = v - v_F$ . Remember that  $v_F = \text{tr}_{\partial T}(v)$ . What we see is for (6) and (9) to be equivalent must this be true.

$$\sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, [u] \rangle_{\partial T} = \sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, u \rangle_{\partial T} - \langle \varepsilon \partial_n u, u_F \rangle_{\partial T} = \sum_{E \in \mathcal{F}^{int}} \varepsilon (\langle \partial_{n^+} u, v_F \rangle_E + \langle \partial_{n^-} u, v_F \rangle). \quad (8)$$

Since  $(u, u_F) \in V$  is has to be continuous, hence the jump is  $[u] = 0$  for the correct solution. Hence, adding  $-\langle \varepsilon \partial_n v, [u] \rangle_{\partial T}$  for symmetry and  $\tau_h \langle \varepsilon [u], [v] \rangle_{\partial T}$  for stability with some stabilization parameter  $\tau_h$  for each  $T \in \mathcal{T}_h$ . This can be added to lhs on (8) such that,

$$\begin{aligned} \sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \{ \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} - \langle \varepsilon \partial_n v, [u] \rangle_{\partial T} + \tau_h \langle \varepsilon [u], [v] \rangle_{\partial T} \} \\ + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} \\ = \sum_{T \in \mathcal{T}_h} (f, v) + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \end{aligned} \quad (9)$$

Finally, we can now construct the discrete system. Let now  $u, u_F \in V_{h,D}$  and  $v, v_F \in V_{h,0}$  be the discretized spaces. Using what we have in (9) can we define

$$\begin{aligned} F(u, u_F, v, v_F) &= \sum_{T \in \mathcal{T}_h} (f, v) + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \\ B(u, u_F, v, v_F) &= \sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \{ \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} - \langle \varepsilon \partial_n [u] \rangle_{\partial T} + \tau_h \langle \varepsilon [u], [v] \rangle_{\partial T} \} + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} \end{aligned}$$

We then end up with the need to solve linear system.

$$B(u, u_F, v, v_F) = F(u, u_F, v, v_F). \quad (10)$$

## 4 $C^0$ Interior Penalty Method

### 4.1 Introduction of the Boundary Value Problem

In this section do we want to establish a numerical method to fourth order equations. Instead of embarking on the special case of surface PDE described in (1) can we establish a general numerical theory on  $\mathbb{R}^2$ , which we later can generalize on closed surface later. Assume that we restrict ourself to a compact surface  $\Omega \in \mathbb{R}^2$  and let  $f \in L^2(\Omega)$  as defined in 5.2. Let say we want to solve the equation on the form.

$$\begin{aligned} \Delta^2 u - \beta \Delta u + \gamma u &= f \quad \beta, \gamma \geq 0 \\ \frac{\partial u}{\partial n} &= 0 \quad \text{on } \Omega \\ \frac{\partial \Delta u}{\partial n} &= q \quad \text{on } \partial \Omega \end{aligned} \quad (11)$$

For convenience are the boundary condition  $q$  chosen to be defined via a  $\phi \in H^4(\Omega)$  such that  $q = \frac{\partial \Delta \phi}{\partial n}$  so  $\frac{\partial \phi}{\partial n} = 0$ .  $\partial \Omega$ .

## 4.2 Weak Formulation

We want to rewrite (11) on weak formulation. Now define the Hilbert space

$$V = \left\{ v \in H^2(\Omega) : \frac{\partial v}{\partial n} = 0 \text{ on } \partial \Omega \right\}.$$

It can be shown [4] that a convinient form is to write it as

$$\begin{aligned} a(u, v) &= (f, v)_{L^2(\Omega)} - (q, v)_{L^2(\partial \Omega)} \\ &= \int_{\Omega} D^2 w : D^2 v dx + \int_{\Omega} \nabla w \nabla v dx + \int_{\Omega} \gamma w \cdot v dx. \end{aligned} \quad (12)$$

For all  $\forall v \in V$ , where

$$D^2 w : D^2 v = \sum_{i,j=1}^2 \frac{\partial^2 w}{\partial x_i \partial x_j} \cdot \frac{\partial^2 v}{\partial x_i \partial x_j}.$$

In fact, according to [4] can it be shown that the problem has a unique solution if and only if  $\gamma > 0$ . However, in the case where  $\gamma = 0$  can we prove a unique solution by introducing the condition

$$\int_{\Omega} f dx = \int_{\partial \Omega} q ds$$

Taking this into account can we expand the solution space such that

$$V^* = \begin{cases} V, & \text{if } \gamma > 0 \\ \{v \in V : v(p^*) = 0\}, & \text{if } \gamma = 0 \end{cases}$$

Where  $p^*$  is a corner in  $\Omega$ . In fact, now all solutions of (12) exists in  $V^*$ .

## 4.3 Construction of $C^0$ Interior Penalty Method

We want to construct a  $C^0$  interior penalty method based on  $C^0$  Lagrange elements. Assume  $\mathcal{T}_h$  be a triangulation of  $\Omega$  and  $V_h$  be the  $\mathcal{P}_2$  Lagrange finite element space associated with  $\mathcal{T}_h$

$$V_h = \left\{ v \in C(\overline{\Omega}) : v_T = v|_T \in \mathcal{P}_2(T) \quad \forall T \in \mathcal{T}_h \right\}$$

So that we can earn a similar space for the approximated solution space ,

$$V_h^* = \begin{cases} V_h, & \text{for } \gamma > 0 \\ \{v \in V_h : v(p^*) = 0\} & \text{for } \gamma = 0. \end{cases}$$

Here is  $p^*$  again a corner in  $\Omega$ . Let us now generalize the Hilbert space as well to the approximated solution space by defining

$$H^k(\Omega, \mathcal{T}_h) = \{H^1(\Omega) : v_T \in H^k(T) \quad \forall T \in \mathcal{T}_h\}.$$

Now assume that that  $e \in \mathcal{E}_h^i$  is shared between two triangles  $T_-, T_+ \in \mathcal{T}_h$ . Then we can assume that the unit normal from  $T_-$  to  $T_+$  is described as  $n_e$  as illustrated in figure 2. Finally, we now want to define jumps internally,

$$\begin{aligned} \left\| \frac{\partial v_h}{\partial n_e} \right\| &= \frac{\partial v_{T_+}}{\partial n_e} \Big|_e - \frac{\partial v_{T_-}}{\partial n_e} \Big|_e, \quad \forall v \in H^2(\Omega, \mathcal{T}_h) \\ \left\| \frac{\partial^2 v_h}{\partial n_e^2} \right\| &= \frac{\partial^2 v_{T_+}}{\partial n_e^2} \Big|_e - \frac{\partial^2 v_{T_-}}{\partial n_e^2} \Big|_e \quad \forall v \in H^3(\Omega, \mathcal{T}_h). \end{aligned}$$

And similarly for means internally,

$$\begin{aligned} \left\| \frac{\partial v_{T_-}}{\partial n_e} \right\| &= \frac{1}{2} \left( \frac{\partial v_{T_+}}{\partial n_e} \Big|_e + \frac{\partial v_{T_-}}{\partial n_e} \Big|_e \right) \quad \forall v \in H^2(\Omega, \mathcal{T}_h) \\ \left\| \frac{\partial^2 v_h}{\partial n_e^2} \right\| &= \frac{1}{2} \left( \frac{\partial^2 v_{T_+}}{\partial n_e^2} \Big|_e + \frac{\partial^2 v_{T_-}}{\partial n_e^2} \Big|_e \right) \quad \forall v \in H^3(\Omega, \mathcal{T}_h), \end{aligned}$$

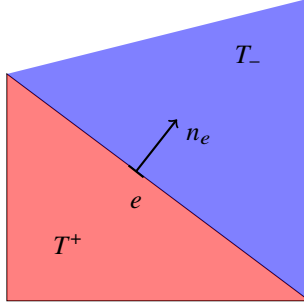


Figure 2: Edge  $e$  shared by the triangles  $T_-$  and  $T_+$  and the normal unit vector  $n_e$ .

Let the edges along the boundary be defined as  $e \in \mathcal{E}_h^b$  along a some boundary triangle  $\mathcal{T}_h$ . We can then define the jump and mean as

$$\begin{aligned} \left[ \left[ \frac{\partial v_h}{\partial n_e} \right] \right] &= -\frac{\partial v_T}{\partial n_e} \Big|_e \quad \forall v \in H^2(\Omega, \mathcal{T}_h) \\ \left\{ \left\{ \frac{\partial^2 v_h}{\partial n_e^2} \right\} \right\} &= \frac{\partial v_T}{\partial n_e} \Big|_e \quad \forall v \in H^3(\Omega, \mathcal{T}_h) \end{aligned}$$

Using the results from [4] can we formulate the discrete formulation the boundary value problem (11) using  $C^0$  interior penalty method. Our goals is to find a  $u_h \in V_h^*$  such that this is true,

$$\mathcal{A}(u_h, v_h) = (f, v_h)_{L^2(\Omega)} - (q, v_h)_{L^2(\partial\Omega)} \quad \forall v_h \in V_h^*. \quad (13)$$

Where  $w_h, v_h \in V_h$  and

$$\begin{aligned} \mathcal{A}(w_h, v_h) &= \sum_{T \in \mathcal{T}_h} \int_T D^2 w_h : D^2 v_h \\ &+ \sum_{e \in \mathcal{E}_h} \int_e \left\{ \left\{ \frac{\partial^2 w_h}{\partial n_e^2} \right\} \right\} \left[ \left[ \frac{\partial v_h}{\partial n_e} \right] \right] ds \\ &+ \sum_{e \in \mathcal{E}_h} \left\{ \left\{ \frac{\partial^2 v_h}{\partial n_e^2} \right\} \right\} \left[ \left[ \frac{\partial w_h}{\partial n_e} \right] \right] ds \quad . \\ &+ \sum_{e \in \mathcal{E}_h} \frac{\sigma}{|e|} \int_e \left[ \left[ \frac{\partial w_h}{\partial n_e} \right] \right] \left[ \left[ \frac{\partial v_h}{\partial n_e} \right] \right] ds \\ &+ \int_{\Omega} \beta \nabla w_h \cdot \nabla v_h dx + \int_{\Omega} \gamma w_h v_h dx. \end{aligned} \quad (14)$$

The notation  $|e|$  is to describe the length of the edge  $e$  and  $\sigma \geq 1$  is a penalty parameter.

## 5 Appendix

### 5.1 The Space $L^2(\Omega)$

Using the definition from [5] and we let  $\Omega$  be an open set in  $\mathbb{R}^d$  and  $p \in \mathbb{R}$  such that  $p \geq 1$ . Then we denote  $L^p(\Omega)$  to be the set of measurable function  $u : \Omega \rightarrow \mathbb{R}$  such that it is equipped in a finite Banach space

$$\|u\|_{L^p(\Omega)} = \left( \int_{\Omega} |u|^p \right)^{\frac{1}{p}}.$$

Now let  $u, v : \Omega \rightarrow \mathbb{R}$ . Then is  $L^2(\Omega)$  a Hilbert space when the inner product is finite such that this exists

$$(u, v)_{L^2(\Omega)} = \int_{\Omega} uv.$$

If the integral is finite do we say that  $u, v \in L^2(\Omega)$ .

### 5.2 The Space $H^m(\Omega)$ , $m > 1$

Again using the definition from [5]. Let  $\alpha = (\alpha_1, \dots, \alpha_d)$ ,  $\alpha \geq 0$ , such that  $|\alpha| = \sum_{i=1}^d \alpha_i$ . Now we define the space

$$H^m(\Omega) = \{u \in L^2(\Omega) : D^\alpha u \in L^2(\Omega) \quad \forall \alpha : |\alpha| \leq m\}.$$

Suppose that  $u, v$  is measurable functions. We can now define  $u \in H^m(\Omega)$  the Banach space is finite.

$$\|u\|_{H^m(\Omega)} = \left( \|u\|_{L^2(\Omega)}^2 + \sum_{k=1}^m \|u\|_{H^k(\Omega)}^2 \right)^{\frac{1}{2}}, \quad \|u\|_{H^k(\Omega)} = \sqrt{\sum_{|\alpha|=k} \|D^\alpha u\|_{L^2(\Omega)}^2}.$$

Similarly for the finite Hilbert space

$$(u, v)_{H^m(\Omega)} = \sum_{|\alpha| \leq m} \int_{\Omega} D^\alpha u D^\alpha v$$

## References

- [1] John W. Cahn and John E. Hilliard. "Free Energy of a Nonuniform System. I. Interfacial Free Energy". In: *The Journal of Chemical Physics* 28.2 (1958), pp. 258–267. DOI: [10.1063/1.1744102](https://doi.org/10.1063/1.1744102). eprint: <https://doi.org/10.1063/1.1744102>. URL: <https://doi.org/10.1063/1.1744102>.
- [2] Vladimir Yushutin et al. "A computational study of lateral phase separation in biological membranes". In: *International Journal for Numerical Methods in Biomedical Engineering* 35.3 (2019). e3181 cnm.3181, e3181. DOI: <https://doi.org/10.1002/cnm.3181>. eprint: <https://onlinelibrary.wiley.com/doi/pdf/10.1002/cnm.3181>. URL: <https://onlinelibrary.wiley.com/doi/abs/10.1002/cnm.3181>.
- [3] Christoph Lehrenfeld. "Hybrid Discontinuous Galerkin methods for solving incompressible flow problems". PhD thesis. May 2010.
- [4] S. Gu and La.). Department of Mathematics Louisiana State University (Baton Rouge. *C0 Interior Penalty Methods for Cahn-Hilliard Equations*. Dissertation (Louisiana State University (Baton Rouge, La.)) Louisiana State University, 2012. URL: <https://books.google.no/books?id=eKP1xQEACAAJ>.
- [5] A. Manzoni, A. Quarteroni, and S. Salsa. *Optimal Control of Partial Differential Equations: Analysis, Approximation, and Applications*. Applied Mathematical Sciences. Springer International Publishing, 2021. ISBN: 9783030772253. URL: <https://books.google.no/books?id=V3NpzgEACAAJ>.