

# Project Thesis

## Solving Cahn Hilliard Equation

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# 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 will 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 $C^0$ Interior Penalty Method

### 3.1 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 4.2. Let say we want to solve the equation on the form.

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

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  $\frac{\partial \phi}{\partial n} = 0$ .  $\partial \Omega$ .

### 3.2 Weak Formulation

We want to rewrite (2) on weak formulation. Now define the Hilbert space

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

It can be shown [3] that a convinient form is to write it as

$$\begin{aligned} a(u, v) &= (f, v)_{L^2(\Omega)} - (q, v)_{L^2(\partial \Omega)} \\ &= \int_\Omega D^2 w : D^2 v \, dx + \int_\Omega \nabla w \cdot \nabla v \, dx + \int_\Omega \gamma w \cdot v \, dx. \end{aligned} \quad (3)$$

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

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

Abusing notation can we see this is clearly arise since

$$\begin{aligned}\int_{\Omega} \Delta^2 w \cdot v dx &= - \int_{\Omega} \nabla (\Delta w) \cdot \nabla v dx \\ &= \int_{\Omega} \Delta w \Delta v dx - \int_{\partial\Omega} \nabla v \frac{\partial \Delta w}{\partial n} ds \\ &= (\Delta w, \Delta v)_{L^2(\Omega)} - (q, v)_{L^2(\partial\Omega)}\end{aligned}$$

why is minus sign in front of  $(q, v)_{L^2(\partial\Omega)}$  and is it correct to use  $q$  in this setting? I also wonder how  $(\Delta w, \Delta v)$  appears to be  $(D^2 w, D^2 v)$  at some point.

In fact, according to [3] 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 provoke 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 (3) exists in  $V^*$ .

### 3.3 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 tringaluation of  $\Omega$  and  $V_h$  be the a  $\mathcal{P}_2$  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

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

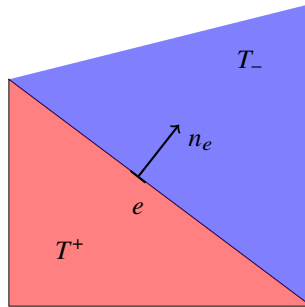


Figure 1: Edge  $e$  shared by the triangles  $T_-$  and  $T_+$  and the normal unit vector  $n_e$ .

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 1. Finally, we now want to define jumps internally,

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

And similarly for means internally,

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

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

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

Using the results from [3] can we formulate the discrete formulation the boundary value problem (2) using  $C^0$  interior penalty method. Our goals is to find a  $u_h \in V_h^*$  such that this is true,

$$\mathcal{A}(u_h, v_h) = (f, v_h)_{L^2(\Omega)} - (q, v_h)_{L^2(\partial\Omega)} \quad \forall v_h \in V_h^*. \quad (4)$$

Where  $w_h, v_h \in V_h$  and

$$\begin{aligned}\mathcal{A}(w_h, v_h) &= \sum_{T \in \mathcal{T}_h} \int_T D^2 w_h : D^2 v_h \\ &\quad + \sum_{e \in \mathcal{E}_h} \int_e \left\langle\left\langle\frac{\partial^2 w_h}{\partial n_e^2}\right\rangle\right\rangle \left[\left[\frac{\partial v_h}{\partial n_e}\right]\right] ds \\ &\quad + \sum_{e \in \mathcal{E}_h} \left\langle\left\langle\frac{\partial^2 v_h}{\partial n_e^2}\right\rangle\right\rangle \left[\left[\frac{\partial w_h}{\partial n_e}\right]\right] ds \\ &\quad + \sum_{e \in \mathcal{E}_h} \frac{\sigma}{|e|} \int_e \left[\left[\frac{\partial w_h}{\partial n_e}\right]\right] \left[\left[\frac{\partial v_h}{\partial n_e}\right]\right] ds \\ &\quad + \int_{\Omega} \beta \nabla w_h \cdot \nabla v_h dx + \int_{\Omega} \gamma w_h v_h dx.\end{aligned} \quad (5)$$

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

## 4 Appendix

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

Using the definition from [4] and we let  $\Omega$  be a 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  $u, v \in L^2(\Omega)$ .

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

Again using the definition from [4]. 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 .

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

Similarly for the finite Hilbert space

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

## References

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