Project Thesis
Solving Cahn Hilliard Equation

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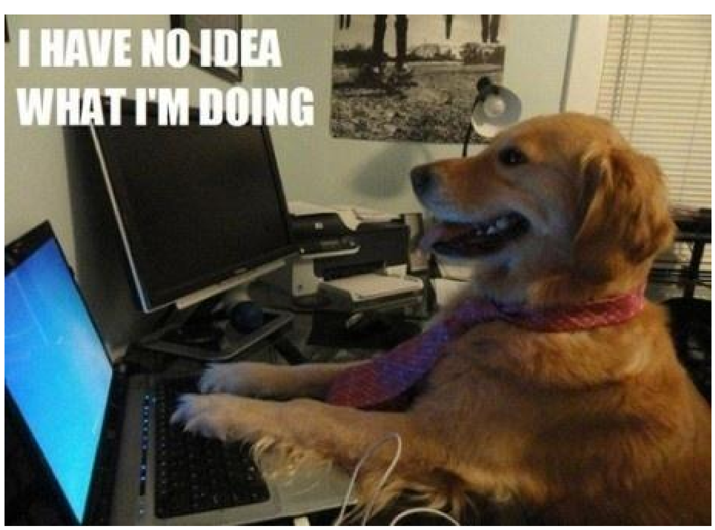

1 Introduction

Introduction

2 Cahn Hilliard Equation on a Closed Membrane

Let c_0 and c_1 indicate the concentration profile of the substances in a a 2 -phase system such that $c_0(\mathbf{x},t) : \Omega\times[0,\infty] \to [0,1]$ and similarly $c_1(\mathbf{x},t) : \Omega\times[0,\infty] \to [0,1]$, where $\mathbf{x}$ is a element of some surface Ω 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 $c(\mathbf{x},t) : \Omega\times[0,\infty] \to [0,1]$. It has been shown that 2 phase system if thermodynamically unstabl can be evolve into a phase seperation described by a evolutional 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 Γ, so that $c(\mathbf{x},t) : \Gamma\times[0,T] \to [0,1]$. Then is the surface Cahn Hilliard equation described such that

$$\rho\frac{\partial c}{\partial t} - \nabla_\Gamma\left(M\nabla_\Gamma\left(f_0' - \varepsilon^2\nabla_\Gamma^2 c\right)\right) = 0 \quad \text{on } \Gamma. \tag{1}$$

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

Lets define ε to be the size of the layer between the substances c_1 and c_2. The density ρ is simply defined such that $\rho = \frac{m}{S_\Gamma}$ is a constant based on the total mass divaded by the total surface area of Γ. Here is the mobility M often derived such that is is dependent on c and is crucial for the result during a possible coarsering 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.

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

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

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

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

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

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 $\left(D^2 w, D^2 v\right)$ 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

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

Where p^* is a corner in Ω. 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 Ω and V_h be the a $\mathcal{P}_2$ Lagrange finite element space associated with $\mathcal{T}_h$

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

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

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

Here is p^* again a corner in Ω. Let us now generelize the Hilbert space as well to the approximated solution space by defining

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

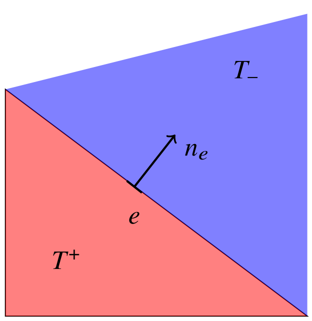

Figure 1: Edge e shared by the triangles T_- and T_+ and the normal unit vector n_e.

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 illustraded in figure 1. Finally, we now want to define jumps internally,

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

And similarly for means internally,

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

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

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

Using the results from [3] can we formulate the discrete formulation the bpundary 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,

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

Where $w_h, v_h \in V_h$ and

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

4 Appendix

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

Using the definition from [4] and we let Ω 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 $u : \Omega \to \mathbb{R}$ 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 $u, v : \Omega \to \mathbb{R}$. Then is $L^2(\Omega)$ a Hilbert space when the inner product is finite such that this exists

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

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

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

Again using the definition from [4]. Let $\alpha = (\alpha_1, \dots, \alpha_d)$, $\quad \alpha \geq 0$, such that $|\alpha| = \sum_{i=1}^d \alpha_i$. Now we define the space

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

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

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

Similarly for the finite Hilbert space

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

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