

Project Thesis

Solving Cahn Hilliard Equation

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1 Introduction

PLAN FOR REPORT

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2 DG for Possion Problem

2.1 Possion Problem

Lets define the problem

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

Here is $\partial\Omega = \Gamma_D \cup \Gamma_N \cup \Gamma_R$.

2.2 Classical DG

2.3 Hybrid DG Method

We want to write this on a weak form. Let the spaces we work on be

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

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,

$$-\sum_{T \in \mathcal{T}_h} \int_T \varepsilon \nabla^2 u \cdot v dx = \sum_{T \in \mathcal{T}_h} \left\{ \int_T \varepsilon \nabla u \cdot \nabla v dx - \int_{\partial T} \varepsilon \cdot \partial_n u \cdot v ds \right\} = \sum_{T \in \mathcal{T}_h} \int_T f \cdot v dx. \quad (1)$$

But we want to introduce the shorter notation equivalently such that

$$\sum_{T \in \mathcal{T}_h} \{ \varepsilon (\nabla u, \nabla v)_T - \varepsilon \langle \partial_n u, v \rangle_{\partial T} \} = \sum_{T \in \mathcal{T}_h} (f, v). \quad (2)$$

Where $\langle \cdot, \cdot \rangle$ is the surface integral operator. Before we continue we want to introduce an 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

$$\sum_{T \in \mathcal{T}_h} \varepsilon \langle \partial_n u, v_F \rangle = \sum_{E \in \mathcal{F}^{int}} \varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E + \sum_{E \in \mathcal{F}^{ext}} \varepsilon \langle \partial_n u, v_F \rangle. \quad (3)$$

Here we are using the definitions n^+ and n^- illustrated using figure 1. Let's define some crucial spaces for the DG method

$$V = \{(u, u_F) : u \in H^2(\mathcal{T}_h) \cap H^1(\Omega), u_F \in L^2(\mathcal{F}_h)\}$$

$$V_h = \{(u, u_F) : u \in \mathcal{P}^k(T) \forall T \in \mathcal{T}_h, u_F \in \mathcal{P}^k(E) \forall E \in \mathcal{F}_h\}$$

and now including dirichlet conditions using the previous definition

$$V_D = \{(u, u_F) \in V, u_F = u_D \text{ on } \Gamma_D\} \quad V_{h,D} = \{(u, u_F) \in V_h, u_F = u_D \text{ on } \Gamma_D\}$$

$$V_0 = \{(u, u_F) \in V, u_F = 0 \text{ on } \Gamma_D\} \quad V_{h,0} = \{(u, u_F) \in V_h, u_F = 0 \text{ on } \Gamma_D\}$$

Defining $(u, u_F) \in V_D$ and $(v, v_F) \in V_0$. Now adding (2) and (3) can we easily see that

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

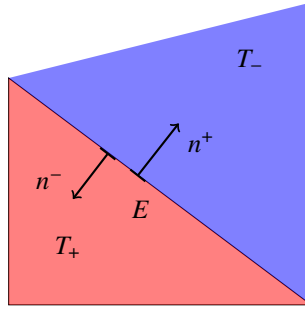


Figure 1: Edge E shared by the triangles T_- and T_+ and the normal unit vectors n^+ and n^- .

Applying the Neumann conditions on Γ_N and Γ_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 $\langle f, v_F \rangle_\Gamma = \int_\Gamma f \cdot v_F \cdot n ds$ for an arbitrary neumann boundary function f on some surface Γ . Hence (4) ends up being

$$\sum_{T \in \mathcal{T}_h} \varepsilon (\nabla u, \nabla v)_T - \sum_{E \in \mathcal{F}^{int}} (\varepsilon \langle \partial_{n^+} u, v_F \rangle_E + \varepsilon \langle \partial_{n^-} u, v_F \rangle_E) + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} = \sum_{T \in \mathcal{T}_h} (f, v)_T + \langle g, v_F \rangle_{\Gamma_N} + \langle h, v_F \rangle_{\Gamma_R}. \quad (5)$$

According to Lehrenfeld 2010 [1] at page 13 on equation (1.2.7) is (5) equivalent to

$$\sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} + \beta \langle \varepsilon u, v_F \rangle_{\Gamma_R} = \sum_{T \in \mathcal{T}_h} (f, v)_T + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R} \quad (6)$$

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 $v_F = tr_{\partial T}(v)$. What we see is for (5) and (6) to be equivalent must this be true.

$$\sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} = \sum_{T \in \mathcal{T}_h} \langle \varepsilon \partial_n u, v \rangle_{\partial T} - \langle \varepsilon \partial_n u, v_F \rangle_{\partial T} = \sum_{E \in \mathcal{F}^{int}} \varepsilon (\langle \partial_{n^+} u, v_F \rangle_E + \langle \partial_{n^-} u, v_F \rangle_E). \quad (7)$$

Since $(u, u_F) \in V$ 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 τ_h for each $T \in \mathcal{T}_h$. This can be added to lhs on (6) such that,

$$\begin{aligned}
& \sum_{T \in \mathcal{T}_h} (\varepsilon \nabla u, \nabla v)_T - \sum_{T \in \mathcal{T}_h} \{ \langle \varepsilon \partial_n u, [v] \rangle_{\partial T} - \langle \varepsilon \partial_n v, [u] \rangle_{\partial T} + \tau_h \langle \varepsilon [u], [v] \rangle_{\partial T} \} \\
& \quad + \beta \langle \varepsilon u, v_f \rangle_{\Gamma_R} \\
& = \sum_{T \in \mathcal{T}_h} (f, v) + \langle \varepsilon g, v_F \rangle_{\Gamma_N} + \langle \varepsilon h, v_F \rangle_{\Gamma_R}
\end{aligned} \tag{8}$$

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 (6) can we define

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

Hence, the numerical method must solve

$$B(u, u_F, v, v_F) = F(v, v_F). \tag{9}$$

3 C^0 Interior Penalty Method for Biharmonic Equation

Let $\Omega \subset \mathbb{R}^2$ be a bounded polygonal domain and $\partial\Omega$ be its corresponding boundary.

Why is this domain chosen to be polygonal?

We can then define the fourth order problem as

$$\begin{aligned} \nabla^4 u - \beta \nabla^2 u + \gamma &= f \quad \text{in } \Omega \\ \partial_n u &= 0 \quad \text{on } \partial\Omega, \\ \partial_n \nabla^2 u &= q \quad \text{on } \partial\Omega \end{aligned} \quad (10)$$

We will assume that γ and β is nonnegative constants, $f \in L_2(\Omega)$, $q = \partial_n \nabla^2 \varphi$, $\partial_n \varphi = 0$ for $\varphi \in H^4(\Omega)$. Such problems as (10) are often associated with the Cahn-Hilliard model [2] for phase separation. As a matter of fact, the major difference is that (10) has no time dependence. However, depending on how Cahn-Hilliard model is time discretized numerically can (10) naturally arise. I refer to [3] for more information on this.

Now, let the solution space be on the form $V = \{v \in H^2(\Omega) : \partial_n v = 0 \text{ on } \partial\Omega\}$ and consider the weak formulation such that we want to solve $u \in V$ such that

$$a(u, v)_\Omega = (f, v)_\Omega - \langle q, v \rangle_{\partial\Omega} \quad \forall v \in V. \quad (11)$$

The inner product has the form

$$a(u, v)_\Omega = \int_\Omega (\nabla^2 w : \nabla^2 v + \beta \nabla w \cdot \nabla v + \gamma w \cdot v) dx.$$

In fact, we must also assume the solvability condition $\int_\Omega f dx = 0$ to obtain a unique solution according [4], [5]. Therefore, can we let the extended solution space

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

where p_* is a corner of the polygonal domain Ω . Thus, the unique solution in $v \in V^*$ belongs to $H^{2+\alpha}(\Omega)$ and we get the following elliptic regularity error estimate,

$$|u|_{H^{2+\alpha}(\Omega)} \leq C_\Omega \left(\|f\|_{L_2(\Omega)} + (1 + \gamma^{\frac{1}{2}}) \cdot \|\varphi\|_{H^4(\Omega)} \right). \quad (12)$$

The constant $\alpha \in (0, 2]$ depends on the interior angles given the corners of Ω , will be referred to as the index of elliptic regularity.

To solve this numerically do we want to introduce the C^0 Interior Penalty Method (C0IP), which is a Discontinuous Galerkin method (DG) using C^0 finite elements. There is several reasons why we want to apply C^0 instead of the often used C^1 finite elements for fourth order problems. First and foremost is the C^0 finite elements simpler than obtaining C^1 finite elements. Also, compared to other methods similar to the mixed finite element method for the problem (10), C0IP has in fact preserved the symmetric positive definiteness, which means the stability analysis is more straight forward. Finally and most importantly according to [3] can naive use mixed methods of splitting the boundary conditions of the problem (10) produce wrong solutions if Ω is nonconvex.

Let $w, v \in H^4(T)$ and \mathcal{T}_h the simplicial triangulation of Ω . We can then define the \mathcal{P}_2 Lagrange finite element spaces so,

$$V_h = \{v \in C(\Omega) : v|_T = v|_T \in \mathcal{P}_2(T), \forall T \in \mathcal{T}_h\}$$

and

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

Using the same method as in [3, 5] can we deduce that for every triangle $T \in \mathcal{T}_h$ is

$$\begin{aligned} (\nabla^4 w, v)_T &= \langle \partial_n \nabla^2 w, v \rangle_{\partial T} - (\nabla(\nabla^2 w), \nabla v)_T \\ &= (D^2 w, D^2 v)_T + \langle \partial_n \nabla^2 w, v \rangle_{\partial T} - \langle \partial_n \nabla w, \nabla v \rangle_{\partial T} \\ &= (D^2 w, D^2 v)_T - \langle \partial_{nt} w, \partial_t v \rangle_{\partial T} - \langle \partial_{nn} w, \partial_n v \rangle_{\partial T} + \langle \partial_n \nabla^2 w, v \rangle_{\partial T} \end{aligned}$$

Need to prove the elliptic regularity conditions.

Simpler than C^1 , in what sense?

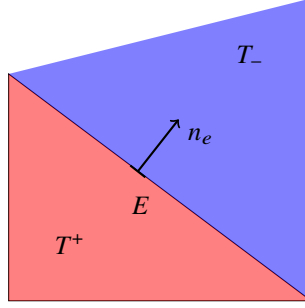


Figure 2: Edge $E \in \mathcal{F}_h$ shared by the triangles $T_+, T_- \in \mathcal{T}_h$ and the normal unit vector n_e .

Keep in mind that this result naturally arise when defining $\nabla = (\partial_n, \partial_t)$ such that

$$\langle \partial_n \nabla w, \nabla v \rangle_{\partial T} = \langle \partial_{nt} w, \partial_t v \rangle_{\partial T} + \langle \partial_{nn} w, \partial_n v \rangle_{\partial T}.$$

Thus, letting $u, v \in H^4(T)$ does this hold for local continuity,

$$(\nabla^4 u, v)_T = (D^2 u, D^2 v)_T - \langle \partial_{nt} u, \partial_t v \rangle_{\partial T} - \langle \partial_{nn} u, \partial_n v \rangle_{\partial T} + \langle \partial_n \nabla^2 u, v \rangle_{\partial T}. \quad (13)$$

For global continuity does it end up with so that $v \in \{v \in H^1(\Omega) : v_T \in H^4(T), \forall T \in \mathcal{T}_h\} \cap C^0(\bar{\Omega})$ such that

$$(\nabla^4 u, v)_\Omega = \sum_{T \in \mathcal{T}_h} (D^2 u, D^2 v)_T + \sum_{E \in \mathcal{F}^{ext}} \langle \partial_n \nabla^2 u, v \rangle_E - \langle \partial_{nt} u, \partial_n v \rangle_E + \sum_{E \in \mathcal{F}^{int}} \langle \partial_{nn} u, \llbracket \partial_n v \rrbracket \rangle_E. \quad (14)$$

What we see is that for (13) and (14) to be equivalent on normal and global form must this be true

$$\sum_{T \in \mathcal{T}_h} -\langle \partial_{nt} u, \partial_t v \rangle_{\partial T} - \langle \partial_{nn} u, \partial_n v \rangle_{\partial T} + \langle \partial_n \nabla^2 u, v \rangle_{\partial T} = \sum_{E \in \mathcal{F}^{ext}} \langle \partial_n \nabla^2 u, v \rangle_E - \langle \partial_{nt} u, \partial_n v \rangle_E + \sum_{E \in \mathcal{F}^{int}} \langle \partial_{nn} u, \llbracket \partial_n v \rrbracket \rangle_E$$

Keep in mind that the jump is defined as $\llbracket \partial_n v \rrbracket = n_e (\nabla v_+ - \nabla v_-)$. We have now the final C0IP formulation,

$$\begin{aligned} \mathcal{A}(w_h, v_h) &= (\beta \nabla w_h \cdot \nabla v_h)_\Omega + (\gamma w_h, v_h)_\Omega \\ &+ \sum_{T \in \mathcal{T}_h} (D^2 w_h, D^2 v_h)_T \\ &+ \sum_{E \in \mathcal{F}_h} \langle \llbracket \partial_{n_e n_e} w_h \rrbracket, \llbracket \partial_{n_e} v_h \rrbracket \rangle_E + \langle \llbracket \partial_{n_e n_e} v_h \rrbracket, \llbracket \partial_{n_e} w_h \rrbracket \rangle_E \\ &+ \tau_h \langle \llbracket \partial_{n_e} w_h \rrbracket, \llbracket \partial_{n_e} v_h \rrbracket \rangle_E \end{aligned} \quad (15)$$

and

$$F(v_h) = (f, v_h)_\Omega. \quad (16)$$

Hence, the discretized numerical problem is to solve $w_h \in V_h$ such that

$$\mathcal{A}(w_h, v_h) = F(v_h), \quad \forall v_h \in V_h.$$

In [5] they introduce

$$\begin{aligned} (D^2 v : D^2 w)_T &= \langle \partial_{nt} v, \partial_t w \rangle_{\partial T} + \langle \partial_{nn} v, \partial_n w \rangle_{\partial T} \\ &= \sum_{i=1}^3 \partial_{n_i t_i} v \int_{E_i} \partial_t w ds + \langle \partial_{nn} v, \partial_n w \rangle_{\partial T} \\ &= \langle \partial_{nn} v, \partial_n w \rangle_{\partial T} \end{aligned}$$

Using the identity $ab + cd = \frac{1}{2}(a+c)(b+d) + \frac{1}{2}(a-c)(b-d)$ they end up with the equations

$$\sum_{T \in \mathcal{T}_h} (D^2 v : D^2 w)_T = - \sum_{E \in \mathcal{F}^{int}} \{ \partial_{n_e n_e} v \} \llbracket \partial_{n_e} w \rrbracket - \llbracket \partial_{n_e n_e} v \rrbracket \{ \partial_{n_e} w \}$$

3.0.1 HC0IP Method copied from NGSolve

We consider the Kirchhoff plate equation: Find $w \in H^2$, such that

$$\int \nabla^2 w : \nabla^2 v = \int f v$$

A conforming method requires C^1 continuous finite elements. But there is no good option available, and thus there is no H^2 conforming finite element space in NGSolve.

$$\sum_T \nabla^2 w : \nabla^2 v - \int_E \{\nabla^2 w\}_{nn} [\partial_n v] - \int_E \{\nabla^2 v\}_{nn} [\partial_n w] + \alpha \int_E [\partial_n w] [\partial_n v]$$

[Baker 77, Brenner Gudi Sung, 2010]

We consider its hybrid DG version, where the normal derivative is a new, facet-based variable:

$$\sum_T \nabla^2 w : \nabla^2 v - \int_{\partial T} (\nabla^2 w)_{nn} (\partial_n v - \widehat{v}_n) - \int_{\partial T} (\nabla^2 v)_{nn} (\partial_n w - \widehat{w}_n) + \alpha \int_E (\partial_n v - \widehat{v}_n)(\partial_n w - \widehat{w}_n)$$

4 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 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 $c(\mathbf{x}, t) : \Omega \times [0, \infty] \rightarrow [0, 1]$. It has been shown that 2 phase system if thermodynamically unstabl can be evolve into a phase seperation described by a evolutional differential equation [2] using a model based on chemical energy of the substances. However, further development has been done [6] 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 $c(\mathbf{x}, t) : \Gamma \times [0, T] \rightarrow [0, 1]$. Then is the surface Cahn Hilliard equation described such that

$$\rho \frac{\partial c}{\partial t} - \nabla_\Gamma (M \nabla_\Gamma (f'_0 - \varepsilon^2 \nabla_\Gamma^2 c)) = 0 \quad \text{on } \Gamma. \quad (17)$$

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 dependent on c and is crucial for the result during a possible coarsening event [6]. However, the free energy per unit surface $f_0 = f_0(c)$ is derived based on the thermodynamical model and should according to [6] be nonconvex and nonlinear.

A important observation is that equation (17) 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.

5 Appendix

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

Using the definition from [7] and we let Ω 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 $u, v \in L^p(\Omega)$.

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

Again using the definition from [7]. 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

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

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