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Abstract

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Declaration

The work in this thesis is based on research carried out at the Department of Computer Science, Durham University, United Kingdom. No part of this thesis has been submitted elsewhere for any other degree or qualification and it is all my own work unless referenced to the contrary in the text.

Acknowledgements

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Contents

List of Figures

List of Tables

Dedication

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CHAPTER 1

Introduction

Let Ω be bounded domain in $\mathbb{R}^d (d \leq 3)$ with Lipschitz boundary $\partial\Omega$. We consider a coupled pair of Cahn-Hilliard Equations modelling a phase separation on a thin film of binary liquid mixture coating substrate, which is wet by one component denoted by A and the other by B:

Find $\{u_1(x,t), u_2(x,t)\} \in \mathbb{R} \times \mathbb{R}$ such that

$$\frac{\partial u_1}{\partial t} = \Delta w_1 \quad \text{in } \ \Omega, t > 0, \tag{1.0.1a}$$

$$\frac{\partial u_2}{\partial t} = \Delta w_2 \quad \text{in } \ \Omega, t > 0, \tag{1.0.1b}$$

where

$$w_1 = \frac{\delta F(u_1, u_2)}{\delta u_1}, \tag{1.0.1c}$$

$$w_2 = \frac{\delta F(u_1, u_2)}{\delta u_2}, \tag{1.0.1d}$$

$$\begin{aligned} F(u_1, u_2) = {} & b_1 u_1^4 - a_1 u_1^2 + c_1 |\nabla u_1|^2 \\ & + b_2 u_2^4 - a_2 u_2^2 + c_2 |\nabla u_2|^2 \\ & + D \left(u_1 + \sqrt{\frac{a_1}{2b_1}} \right)^2 \left(u_2 + \sqrt{\frac{a_2}{2b_2}} \right)^2 . \end{aligned} \tag{1.0.1e}$$

Here $\delta F(u_1, u_2)/\delta u_i$, for $i = 1, 2$, indicates the functional derivative. The variable u_1 denotes a local concentration of A or B and u_2 indicates the presence of a liquid or a vapour phase. c_i denote the surface tension of u_i. The coefficient a_i is proportional to $T_{c_i} - T$, where T_{c_1} corresponds to the critical temperature of the A-B phase separation, and T_{c_2} represents the critical temperature of the liquid-vapour phase separation.

If $a_1 > 0$, $a_2 > 0$, there are two equilibrium phases for each field corresponding to $u_1 = \pm\sqrt{\frac{a_1}{2b_1}}$ and $u_2 = \pm\sqrt{\frac{a_2}{2b_2}}$, denote as u_1^+, u_1^-, u_2^+, and u_2^-. The coupling D energetically inhibits the existence of the phase denoted by the $(u_1^+,\, u_2^+)$. Thus we have three-phase system: liquid A correspond to $(u_1^-,\, u_2^-)$ regions, liquid B to $(u_1^+,\, u_2^-)$ regions and the vapour phase to $(u_1^-,\, u_2^+)$ regions.

If $D = 0$, the problem reduces to two decoupled Cahn-Hilliard equations, which has been discussed at length in the mathematical literature. And for this type of problem, we do not have liquid-vapour interfaces.

In Chapter 5 two practical algorithms (implicit an explicit methods) for solving the finite element at each time step are suggested. We discuss the convergence theory for the implicit scheme, which used to solve the system arising from Scheme 1. We also discuss in this chapter some computational results for one and two space dimensions. We only use the implicit scheme for all simulations. Before showing some computational results, we discuss linear stability solutions in one space dimension.

CHAPTER 2

Evolutionary problem

In this chapter a global existence and uniqueness theorem for a weak formulation possessing a Lyapunov function is proven. Regularity results are presented for the weak solution.

2.1 Notation

Let Ω be a bounded domain in $\mathbb{R}^d,\ d \leq 3$ with boundary $\partial\Omega$. For $d = 2, 3$ we assume that $\partial\Omega$ is Lipschitz boundary. Through out this thesis we adopt the standard notation for Sobolev spaces, denoting the norm of $W^{m,p}(\Omega)\,(m \in \mathbb{N}, p \in [1, \infty])$ by $\|\cdot\|_{m,p}$ and semi-norm by $|\cdot|_{m,p}$. For $p = 2$, $W^{m,p}(\Omega)$ will be denoted by H^m with the associated norm and semi-norm written as $\|\cdot\|_m$ and $|\cdot|_m$, respectively. In addition we denote the $L^2(\Omega)$ inner product over Ω by $(\cdot, \cdot)$ and define the mean of integral

$$\fint \eta := \frac{1}{|\Omega|}(\eta, 1) \quad \forall \eta \in L^1(\Omega).$$

We also use the following notation, for $1 \le q < \infty$,

$$L^q(0,T;W^{m,p}(\Omega)) := \left\{ \eta(x,t) : \ \eta(\cdot,t) \in W^{m,p}(\Omega), \int_0^T \|\eta(\cdot,t)\|_{m,p}^q \, dt < \infty \right\},$$
$$L^\infty(0,T;W^{m,p}(\Omega)) := \left\{ \eta(x,t) : \eta(\cdot,t) \in W^{m,p}(\Omega), \ \operatorname*{ess\,sup}_{t\in(0,T)} \|\eta(\cdot,t)\|_{m,p} < \infty \right\},$$

For later purposes, we recall the Hölder inequality for $u \in L^p$, $v \in L^q$ and $1 < p < \infty$,

$$\int_\Omega |uv| dx \le \left(\int_\Omega u^p dx \right)^{\frac{1}{p}} \left(\int_\Omega v^q dx \right)^{\frac{1}{q}}, \quad \text{where } \frac{1}{p} + \frac{1}{q} = 1, \tag{2.1.1}$$

and the following well-known Sobolev interpolation results: Let $p \in [1,\infty]$, $m \ge 1$ and $v \in W^{m,p}(\Omega)$. Then there are constants C and $\mu = \frac{d}{m}\left(\frac{1}{p} - \frac{1}{r}\right)$ such that the inequality

$$|v|_{0,r} \le C|v|_{0,p}^{1-\mu} \|v\|_{m,p}^{\mu}, \quad \text{holds for } r \in \begin{cases} [p,\infty] & \text{if } m - \frac{d}{p} > 0, \\ [p,\infty) & \text{if } m - \frac{d}{p} = 0, \\ [p, -\frac{d}{m-d/p}] & \text{if } m - \frac{d}{p} < 0. \end{cases} \tag{2.1.2}$$

We also state the following lemma, which will prove useful in our subsequent analysis.

Lemma 2.1.1 Let $u, v, \eta \in H^1(\Omega)$, $f = u - v$, $g = u^m v^{n-m}$, $m, n = 0, 1, 2$, and $n - m \ge 0$. Then for $d = 1, 2, 3$,

$$\left| \int_\Omega f g \eta dx \right| \le C|u - v|_0 \, \|u\|_1^m \, \|v\|_1^{n-m} \, \|\eta\|_1. \tag{2.1.3}$$

Proof: Note that using the Cauchy-Schwarz inequality we have

$$|(u)^m v^{n-m}|_{0,p} \le \begin{cases} |u|_{0,2mp}^m \, |v|_{0,2(n-m)p}^{(n-m)} & \text{for } \ n - m \ne 0, \ \text{ and } \ m \ne 0, \\ |u|_{0,mp}^m \ \text{ or } \ |v|_{0,(n-m)p}^{(n-m)} & \text{for } \ m = 0, \ \text{ or } \ n - m = 0 \ \text{ respectively.} \end{cases}$$

Noting the generalise Hölder inequality and the result above we have

$$
\begin{aligned}
\left| \int_\Omega fg\eta dx \right| &\leq |u-v|_0 \; |u^m v^{n-m}|_{0,3} \; |\eta|_{0,6}, \\
&\leq |u-v|_0 \;\; |\eta|_{0,6} \begin{cases} |u|_{0,6}^2 & \text{for } \; m=2, \\ |u|_{0,6} \; |v|_{0,6} & \text{for } \; m=1, \\ |v|_{0,6}^2 & \text{for } \; m=0, \end{cases} \\
&\leq C|u-v|_0 \; \|u\|_1^m \; \|v\|_1^{n-m} \; \|\eta\|_1,
\end{aligned}
$$

where we have noted ([**?**]) to obtain the last inequality. This ends the proof. □

2.2 The Existence and Uniqueness of the Continuous Problem

Given $\gamma > 0$ and $u_i^0 \in H^1(\Omega)$, for $i = 1, 2$, such that $\|u_1^0\|_1 + \|u_2^0\|_1 \leq C$. We consider the problem:

(**P**) Find $\{u_i, w_i\}$ such that $u_i \in H^1(0,T;(H^1(\Omega))') \cap L^\infty(0,T;H^1(\Omega))$ for *a.e.* $t \in (0,T)$, $w_i \in L^2(0,T;H^1(\Omega))$

$$\left\langle \frac{\partial u_1}{\partial t}, \eta \right\rangle = -(\nabla w_1, \nabla \eta), \tag{2.2.1a}$$

$$(w_1, \eta) = (\phi(u_1), \eta) + \gamma(\nabla u_1, \nabla \eta) + 2D(\Psi_1(u_1, u_2), \eta), \tag{2.2.1b}$$

$$u_1(x, 0) = u_1^0(x), \tag{2.2.1c}$$

and

$$\left\langle \frac{\partial u_2}{\partial t}, \eta \right\rangle = -(\nabla w_2, \nabla \eta), \tag{2.2.1d}$$

$$(w_2, \eta) = (\phi(u_2), \eta) + \gamma(\nabla u_2, \nabla \eta) + 2D(\Psi_2(u_1, u_2), \eta), \tag{2.2.1e}$$

$$u_2(x, 0) = u_2^0(x), \tag{2.2.1f}$$

for all $\eta \in H^1(\Omega)$ for *a.e.* $t \in (0,T)$.

CHAPTER 3

A Semidiscrete approximation

In this chapter we introduce some notation which will be used in the current and following chapters. For completeness, we prove interpolation error estimates in the finite element space as these are necessary tools for analysis the current chapter and chapter 4. Then a semidiscrete finite element approximation is proposed where the existence is shown and the uniqueness is proven for one and two dimensions. An error bound between the semidiscrete and continuous solution is given is the final section.

3.1 Notations

Let $S^h \subset H^1(\Omega)$ be finite element space defined by

$$S^h := \{\chi \in C(\bar{\Omega}) : \chi|_\tau \text{ is linear } \forall \tau \in \mathcal{T}^h\} \subset H^1(\Omega).$$

Denote by $\{x_i\}_{i=1}^J$ the set of nodes of $\mathcal{T}^h$ and let $\{\eta_i\}_{i=1}^J$ be basis for S^h defined by $\eta_i(x_j) = \delta_{ij}$, for $i, j = 1, \ldots, J$.

Let $\pi^h : C(\bar{\Omega}) \mapsto S^h$ be the interpolation operator such that $\pi^h \chi(x_i) = \chi(x_i)$, for $i = 1, \ldots, J$ and define a discrete inner product on $C(\bar{\Omega})$ as follows

$$(\chi_1, \chi_2)^h := \int_\Omega \pi^h(\chi_1(x)\chi_2(x))dx \equiv \sum_{i=1}^{J} m_i \chi_1(x_i)\chi_2(x_i), \tag{3.1.1}$$

where $m_i = (\eta_i, \eta_i)^h$. The induced norm $\|\cdot\|_h := [(\cdot,\cdot)^h]^{\frac{1}{2}}$ on S^h is equivalent to $|\cdot|_0 := [(\cdot,\cdot)]^{\frac{1}{2}}$. Note that the integral ([**?**]) can easily be computed by means of vertex quadrature rule, which exact for piecewise linear functions.

CHAPTER 4

A fully discrete approximation

In this chapter we introduce a numerical scheme (we call scheme 1) to solve the weak formulation form we mentioned in Chapter 1. We discussed the existence and uniqueness of the solutions for the scheme. We also discuss stability and convergence of the solution to the continuous problem in the weak formulation. We briefly mention a second scheme (we call scheme 2) and show existence, uniqueness, and the stability. We do not discuss the convergence of the scheme.

4.1 Scheme 1

4.1.1 Existence and Uniqueness

Given N, a positive integer, let $\Delta t = T/N$ denote a fixed time step, and $t^k = k\Delta t$ where $k = 0, \ldots, N$. We focus our attention on approximating $(\mathbf{P})$ by the discrete scheme defined as follows:

$(\mathbf{P}_1^{h,\Delta t})$ Given U_1^0, U_2^0, find $\{U_1^n, U_2^n, W_1^n, W_2^n\} \in S^h \times S^h \times S^h \times S^h$, for $n = 1, \ldots, N$, such that $\forall \eta \in S^h$

$$(\frac{U_1^n - U_1^{n-1}}{\Delta t}, \eta)^h = -\,(\nabla W_1^n, \nabla \eta), \tag{4.1.1a}$$

$$(W_1^n, \eta)^h = (F_1(U_1^n, U_2^n), \eta)^h + \gamma(\nabla U_1^n, \nabla \eta), \tag{4.1.1b}$$

$$U_1^0 = P^h u_1^0, \tag{4.1.1c}$$

and

$$(\frac{U_2^n - U_2^{n-1}}{\Delta t}, \eta)^h = -\,(\nabla W_2^n, \nabla \eta), \tag{4.1.1d}$$

$$(W_2^n, \eta)^h = (F_2(U_1^n, U_2^n), \eta)^h + \gamma(\nabla U_2^n, \nabla \eta), \tag{4.1.1e}$$

$$U_2^0 = P^h u_2^0, \tag{4.1.1f}$$

where

$$F_1(U_1^n, U_2^n) = (U_1^n)^3 - U_1^{n-1} + D(U_1^n + U_1^{n-1} + 2)(U_2^{n-1} + 1)^2, \tag{4.1.1g}$$

$$F_2(U_1^n, U_2^n) = (U_2^n)^3 - U_2^{n-1} + D(U_2^n + U_2^{n-1} + 2)(U_1^n + 1)^2. \tag{4.1.1h}$$

Note that (**??**–c) is independent of U_2^n and (**??**–f) is dependent on U_1^n.

CHAPTER 5

Numerical Experiments

In this chapter we discuss two practical algorithms (implicit and explicit method) that are used to solve an algebraic system arising in the problem discussed in this thesis. We discuss the convergence theory for the implicit scheme as used to solve the system arising from the scheme 1. We also discuss some computational results for one and two dimensions. We use the implicit scheme in all simulations in this chapter. We have made a comparison with Scheme 2 and the results are compatible. Before showing some computational results, we discuss linear stability solution for the problem.

5.1 Practical Algorithms

5.1.1 Iterative Method for Scheme 1

Let us expand U_i and W_i, $i = 1, 2$, in terms of the standard nodal basis functions of the finite element space S^h, that is,

$$U_1^n = \sum_{i=1}^{J} U_{1,i}^n \eta_i, \quad W_1^n = \sum_{i=1}^{J} W_{1,i}^n \eta_i, \tag{5.1.1a}$$

$$U_2^n = \sum_{i=1}^{J} U_{2,i}^n \eta_i, \quad W_2^n = \sum_{i=1}^{J} W_{2,i}^n \eta_i, \tag{5.1.1b}$$

where J be the number of node points.

Concluding Remarks

To see a clear interaction between the solutions U_1 and U_2 in terms of their physical meaning, it is worthwhile doing computational experiment in three space dimensions.

CHAPTER 6

Conclusions

It was shown using a Faedo Galerkin approximation that there exist a unique solution for the coupled pair of Cahn-Hilliard equations modelling a phase separation on a thin film of binary liquid mixture coating substrate, which is wet by one component. This solution satisfies certain stability bounds. The regularity result was driven at the end of Chapter 2 as having major contribution in obtaining the error bound for the method proposed.