ABSTRACT

ALANEZY, KHALID ALI. Optimal Control of Moving Interface and Phase-Field Separations. (Under the direction of Kazufumi Ito.)

In this thesis we consider two moving interface problems of practical interests. The first one is the sharp interface model of solidification by the classical two-phase Stefan problem, and the second one is the phase-field model by the coupled Cahn-Hilliard Navier-Stokes system. The main objective of this thesis is to formulate the optimal control problem for the motion of the change of phase and phase separation of the binary fluid mixture by the boundary control. The Lagrange calculus is used in the analysis of the two highly non-linear and non-smooth control problems. Phase changing and phase separation are considerably involved with a lot of applications in industry.

For the case of two-phase Stefan problem, our objective is to control the motion of the solidification interface by formulating a tracking type optimal control problem. The control we use is the heat flux at a portion of the boundary, so that we achieve a desired solidification motion by the boundary control.

For the Cahn-Hilliard Navier-Stokes system, our main goal is to control the separation of the two fluids by the boundary control of the fluid velocity field. The Navier-Stokes equations are coupled to the Cahn-Hilliard system in the following way. The velocity field introduces the transport term of the concentrations in the Cahn-Hilliard equations, the fluid structure interaction force is added into the incompressible Navier-Stokes equations as an interaction force, and our control enters as a Dirichlet boundary condition for the velocity field.

In both models, we will study the well-posedness of the problem, i.e. we will introduce the weak form of equations and then show the existence of weak solutions as well as proving the Lipschitz continuity of solutions with respect to control and initial conditions. Lastly, we will develop numerical methods with control to construct the optimal boundary control based on the so-called Sequential Programing method.

Optimal Control of Moving Interface and Phase-Field Separations

by
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DEDICATION

To my beloved parents, my wife and my children.

BIOGRAPHY

The author was born in 1986 in Saudi Arabia, and raised with his three brothers and five sisters. He is married and has two sons and one daughter.

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Chapter 1

Introduction

In this thesis we will study two important moving interface problems of practical interests. In particular, we will focus on control of the interface motion. The first problem is the sharp interface model of solidification by the classical two-phase Stefan problem [10, 41, 42, 15, 44]. The second one is the phase-field model for the separation of two fluids by the coupled Cahn-Hilliard Navier-Stokes system [2, 4, 18, 31, 12]. Those two problems are related to each other, since the limit of the phase-field model is given by the sharp interface model.

Our objective is to introduce a mathematical formulation of the two models based on variational approach using the corresponding energy functional. Most importantly, our analysis is developed for each model with boundary control. Then, we formulate the optimal control problem for each case and derive the necessary optimality condition. Based on the optimality condition, we develop numerical algorithms to find the optimal control. The analysis of those two problems helps us to promote the study of different moving interface problems.

The classical two-phase Stefan problem is one of the fundamental mathematical models of solidification processes of different materials, such as aluminum [9], and steel [34]. It is a sharp interface model which determines the motion of the interface by the so called free boundary problem. The equation is named after the physicist Jožef Stefan who worked on this problem in 1890 and published a series of papers in which he considered the process of seawater freezing. The standard two-phase Stefan problem is governed by the parabolic heat equation formulated for the solid and liquid phases coupled with the motion of the interface, which is assumed to be a surface separating the two different phases. We assume that the temperature at the interface equals the solidification temperature. The mechanism determining the evolution of the free boundary between the two phases uses the difference of flux along the free boundary for the evolution of the interface.

The two-phase Stefan model is widely used in the field of industry. For example, it is used in the freeze-cast method which is utilized to make porous ceramics [57]. In industry fields, they first prepare ceramic slurry and then freeze it on a cold surface to produce the desired ceramic. Porous ceramics have low thermal conductivity and therefore they are utilized in filters, thermal insulation and energy devices. The process of making porous ceramics begins by pouring the slurry into a mould which undergoes isotropic cooling to induce solidification, as shown in Figure (1.1). In order to have certain mechanical properties of pore networks of freeze

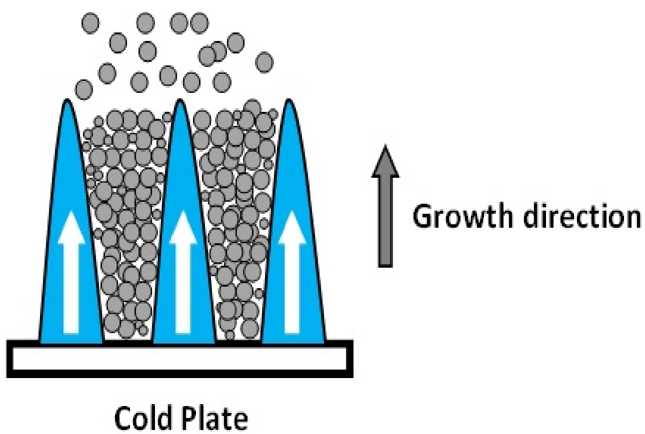

Figure 1.1 Freeze cast process

cast ceramics, we focus mainly on porosity and pore size. Pore size decreases with increasing freezing front velocity, i.e. the speed at which the solid-liquid interface advances. The interface velocity increases with decreasing freezing surface temperature. To be able to use freeze cast products commercially, we need to have a specially designed casting setup in which we can determine processing conditions that gives a set of pore network characterizations a priori. Since pore size is determined by velocity of freezing front, a pore size model must include an effective method to predict the velocity of freezing interface which can be achieved using the two-phase Stefan model. The importance of determining solidification front velocity arises in different industrial processes such as metal casting and crystal growth.

In order to motivate our objective, i.e. formulate the optimal control problem for the motion of the moving interface by the boundary control, Figure (1.2) below shows how (fixed in time control) achieves solidification of solid region by boundary heat flux. In the figure, we have a solid region (dark blue), surrounded by a liquid region (light blue) and a boundary heat flux at a portion of the boundary Γ_c. After some time, we see the evolution of the interface region, which leads to shrinking of the solid region till the solid region splits into two pieces. Our control can be accomplished by tracking a desired interface motion and constructing the cost functional in which we regulate the difference between the graph of the physical interface and the desired interface [10, 41, 42]. The control uses the flux at a portion of the exterior boundary to design the motion of the interface.

In the classical approach based on the two phase Stefan problem, we must determine the motion of the interface Γ_t along with the solutions to heat equations on each phase via the interface condition. But we use the equivalent formulation of the Stefan problem based on the enthalpy formulation. The enthalpy is the total thermal energy and is a monotone piecewise linear function of temperature. The enthalpy satisfies the nonlinear (non-smooth but monotone) heat equation with boundary heat flux control. The control enters into the equation as the boundary heat flux control on a portion of the boundary. During the process of phase changing, a latent heat is either released out or absorbed by the system at the interface. The latent heat exchange causes a discontinuity (or a jump) on the enthalpy at a critical solidification temperature, and yields to a thickness of the interface layer [8, 9]. One can derive the weak form of the enthalpy equation in which the boundary control appears naturally as the boundary integral in the weak form. Then, we study the existence and regularity properties of weak solution for the enthalpy formulation, e.g. see [46, 64, 20]. The temperature is then determined as a function of the enthalpy. The advantage of the enthalpy formulation is that it is more effective to develop the mathematical formulation with boundary control and also develop numerical analysis for the solutions of the problem.

The second problem is the physical phenomena of phase separation of a binary fluid mixture. We use the Cahn-Hilliard equation as a mathematical model for the phase separation. The two components could refer, for example, to water and oil. When an alloy, that is a mixture of two metallic components, is heated, and then cooled quickly to a lower temperature, a phase separation can occur suddenly. This separation of the metal alloy into two components, by lowering the temperature of the mixture, is known as spinodal decomposition [14].

The equation is named after John Cahn and John Hilliard who proposed this equation in 1958. The Cahn-Hilliard equation explains the dynamics of the separation of two fluids into two separate pure phases [28]. John Cahn and John Hilliard began work on the spinodal decomposition problem in the late 1950s. In particular, they considered a molten iron-nickel alloy [13]. Their goal was to describe how the alloy separates into its two components. By suddenly dropping the temperature of the alloy, very small formations of pure iron and pure

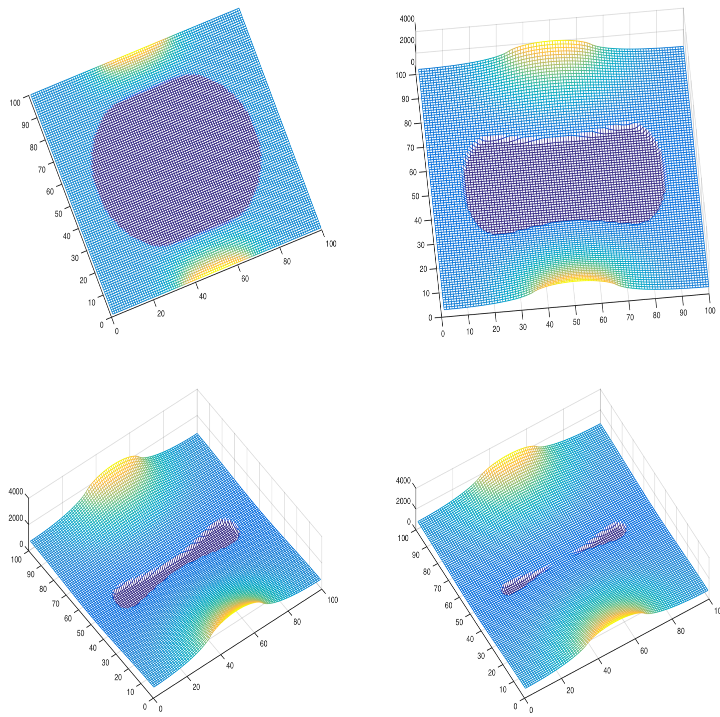

Figure 1.2 Splitting of solid region (blue) by boundary flux

nickel appears. After some time, these formation of pure phases coarsen into larger ones. It is very important to understand the dynamic of the formation of this coarsen regions which leads to the process of separating the two components. The separation process of the two components occurs along with pattern formation and evolution.

One of the important practical applications of Cahn-Hilliard Navier-Stokes equations is the refining of aluminum by removing magnesium particles from molten aluminum alloys [58]. The production of aluminum alloys is very useful in mechanic automotive and aerospace components industry, mainly since aluminum has low density and high corrosion resistance. However, to use those alloys in industry, they must not contain more than 0.1 % magnesium. There are several methods to recycle aluminum alloys and get rid of magnesium particles. The most cost effective and environmentally friendly method of aluminum recycling is the so called submerged injection of silica particles with argon as carrier gas in aluminum alloys. This removal process is called gas-injection treatment, where gas is being injected into the molten alloy, as shown in Figure (1.3). To model the particles trajectories and mass transfer in powder injection processes, we need to

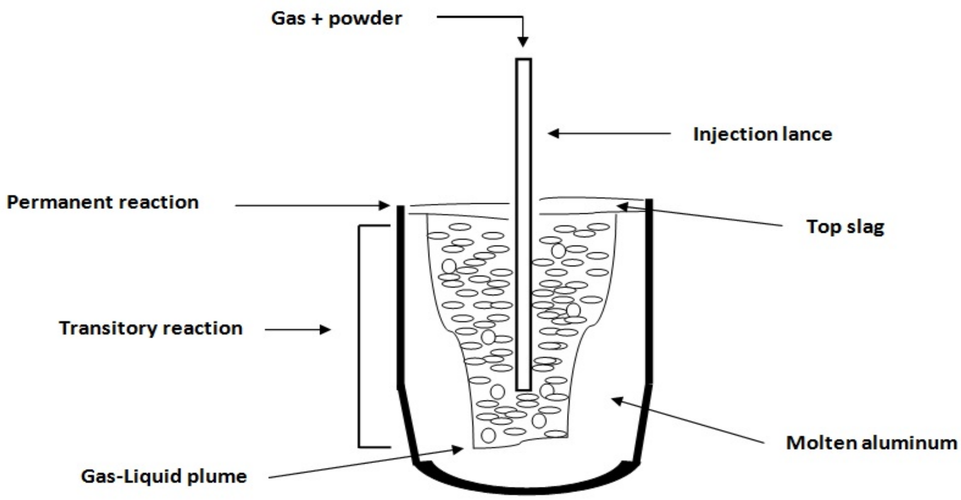

Figure 1.3 Submerged gas injection into metallurgical refining process

have a quantitative information of gas-liquid flow. Thus, the diffuse interface method is used to predict the behavior of argon gas injection into the molten aluminum. The Computational fluid dynamics modeling for injection process is formulated by using the coupled Cahn-Hilliard Navier-Stokes system. The system describes the flow induced by the argon gas and models the dynamic evolution of the interface layer between gas plume and liquid metal. In the diffuse interface methods, the evolution of the interfacial layer is governed by a phase-field variable c that obeys the convective-diffusion Cahn-Hilliard equation.

Our objective in this thesis for the Cahn-Hilliard Navier-Stokes system is to control the separation of a binary fluid mixture by the boundary control of the fluid velocity field. To motivate our objective, Figure (1.4) shows the simulation of the rotating velocity field to coarsen regions of pure phases during the separation process. The figure shows a mixture of two fluids (yellow and blue dots), then if we apply a rotating velocity field to the mixture, then a very small formations of pure liquids appear. After some time, these formations of pure phases coarsen into larger ones. The dynamic of the formation of this coarsen regions leads to the separation of the two components. The Cahn-Hiiliard theory uses H^{-1} gradient flow based on the free energy with the Ginzburg-Landau potential [27]. The Navier-Stokes equation is coupled with the Cahn-Hiiliard equation, i.e., the velocity field introduces the transport term in the Cahn-Hiiliard equation and the fluid-structure force is added to the incompressible Navier-Stokes equations and control enters as a Dirichlet boundary condition for the velocity filed. The coupling should

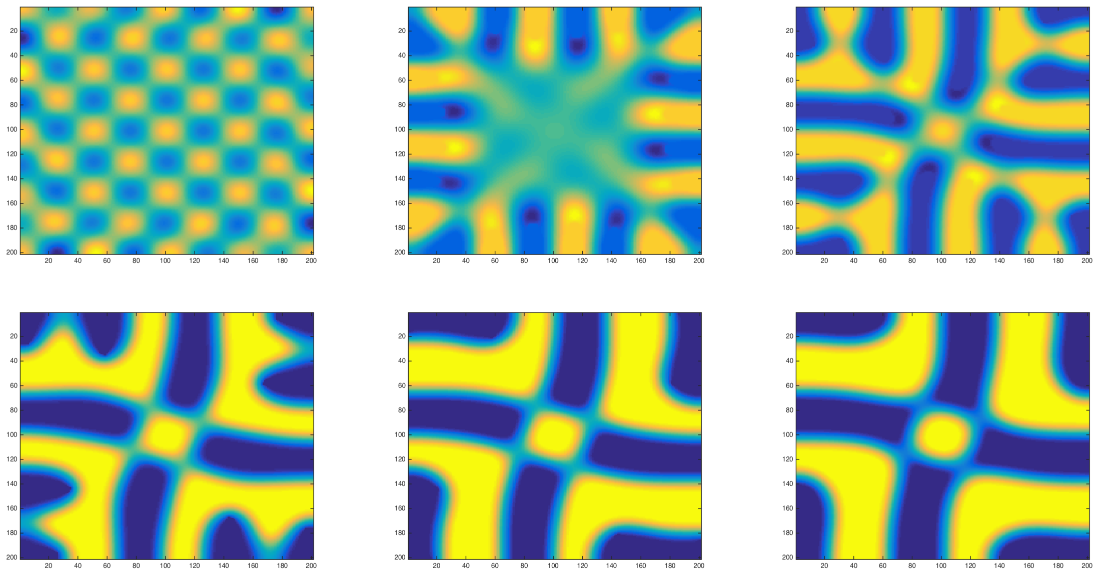

Figure 1.4 Separation with rotating velocity field

control the separation indirectly based on Cahn-Hiiliard Navier-Stokes model. Because of the fluid-structure interaction force, we can control the fluid by the boundary control of the fluid [38, 39]. Examples of control actions include sliding, rotation, injection and sucking. Understanding the dynamic of the separation has been the subject of much research in the 20th century [27].

The plan of this thesis is as follows. In Chapter 2 we focus on the solidification problem. First, we develop the variational formulation of enthalpy equation with boundary control, based on the thermal energy for the two phase Stefan problem and the corresponding weak form of equations [59, 19, 24]. Second, we show the existence of weak solutions with the help of Aubin's lemma. Then, we prove the Lipschitz continuity of solutions with respect to boundary control and initial conditions.

In Chapter 3 we formulate the optimal boundary control problem of tracking the desired motion for the solidification interface and show the existence of optimal control. Next, we derive the necessary optimality using the Lagrange calculus. We also develop numerical discretization method with control to construct the optimal boundary control based on the sequential programing for the necessary optimality condition [47]. Lastly, we present some numerical test examples for achieving a desired solidification.

In Chapter 4 we study the Cahn-Hiiliard Navier-Stokes equations. First, we develop the variational formulation of the Cahn-Hiiliard Navier-Stokes control system, based on the free energy formulation and the corresponding weak form of equations [51, 36]. Second, we show the existence of weak solutions. We also prove the Lipschitz continuity of solutions with respect to velocity control and initial conditions using the Galerkin approach and Aubin's lemma for the compactness of Galerkin solutions. We use semi-group theory to lift regularity of concentration c. Also, we consider the sharpened Ginzburg-Landau potential as in [36, 37] as a specific model for our analysis and numerics. As done in [36], we obtain the chemical potential for the obstacle potential, i.e. the concentration c is constrained to $|c| \leq 1$, for the phase separation in terms of the L^2-multiplier and the complementary condition.

In Chapter 5 we formulate the optimal boundary control problem of tracking a desired state. We derive the necessary optimality using Lagrange calculus. We also develop numerical methods with control to construct the optimal boundary control.

For the optimal control problems in both models, it is not straight forward to apply directly the standard Lagrange multiplier theory [47], since we need to introduce function spaces which are different from Gelfand-triple formulation. Thus, we use the so-called Lagrange calculus approach, as in [47], to derive the necessary optimality. The details of Lagrange calculus approach are described in Appendix B.

In the numerical analysis, we discretize the energy in a lattice for both problems. For the two-phase Stefan problem, the energy is represented by enthalpy, while for Cahn-Hilliard system, the energy is represented by the free potential energy in terms of the concentration c. A specific form of the sequential programing is discussed in Appendix D.2, and the details of algorithmic aspects of the conjugate gradient implementation are described in the Appendix D.3.

Chapter 2

The Classical Two-Phase Stefan Problem

In this chapter we focus on the classical two-phase Stefan problem. First, we introduce the enthalpy formulation of the problem. Then, we derive the differential form of the two-phase Stefan model based on the enthalpy formulation. Next, we show the existence of weak solutions of the enthalpy formulation with the help of Aubin's lemma. We also prove Lipschitz continuity of solutions with respect to control and initial conditions.

Stefan problem is a moving interface model that describes change of phase, as in, for example, solidification or melting of ice. The change of phase occurs in a mushy zone, called the interface, where the liquid and solid phases are present simultaneously. The model has important applications in natural sciences and industrial processes [61], as described in the introduction.

2.1 Enthalpy Formulation of the Two-Phase Stefan Problem

In the classical temperature formulation of the two-phase Stefan problem, the location of the moving interface has to be determines as part of the solution and cannot be identified in advanced. Therefore, solutions based on this formulation become difficult to analyze, especially in multidimensional problems. Alternatively, there have been many formulations developed to analyze free boundary problems. The enthalpy method is widely used in solving the two-phase Stefan problem as it reformulates the heat conduction equation to involve the internal energy represented by enthalpy without the need to regard the motion of the interface as an explicit boundary condition.

In this section we introduce the enthalpy formulation to study the two-phase Stefan problem.

Enthalpy, as a function of temperature, is a measurement of energy in a thermodynamic system. It is the thermodynamic quantity equivalent to the total heat content of a system, i.e. the sum of the specific heat and the latent heat. Recall that the standard single-phase heat conduction equation with flux control g is given by

$$E_t = (\rho c\theta)_t = \kappa\Delta\theta, \qquad \kappa\frac{\partial\theta}{\partial\nu} = g, \tag{2.1}$$

where $\theta(x,t)$ is the temperature at any point $x \in \Omega$ and time $t > 0$, E is the enthalpy given by $E = \rho c\theta$. Here $\rho(x) > 0$ is the mass density, $c = c(\theta)$ is the specific heat, as a function of θ, and g is the flux control at portion of the boundary Γ_c. The specific heat can be defined as the amount of heat per unit mass required to raise the temperature by one degree Celsius.
Now, we introduce the enthalpy law for dual-phase, i.e. solid and liquid. The difference between the single phase and dual phases, that the enthalpy has a jump at a critical solidification temperature T_m with jump size ρL, due to latent heat exchange. The latent heat L is defined as the energy released or absorbed by a thermodynamic system. This jump condition is often called Stefan condition. In Figure (2.1), one can see the enthalpy graph [20, 8, 61], defined as,

$$\gamma(T) = \begin{cases} \rho c_\ell(T - T_m) + \rho L, & T \geq T_m, \\ [0, \rho L], & T = T_m, \\ \rho c_s(T - T_m), & T \leq T_m. \end{cases} \tag{2.2}$$

where $T = \theta$ is the temperature, ρ is the mass density of solid and liquid, c_s, c_l are specific heat of solid and liquid, respectively, and L is the latent heat.
On the other hand, the inverse of the set-valued graph γ, defined by (2.2) is $\theta = \beta(E)$, a function of the enthalpy as in Figure (2.2). That is,

$$\beta(E) = \begin{cases} T_m + \dfrac{1}{\rho c_\ell}(E - \rho L), & E \geq \rho L, \\ T_m, & 0 \leq E \leq \rho L, \\ T_m + \dfrac{1}{\rho c_s}E, & E \leq 0. \end{cases} \tag{2.3}$$

Observe that $\theta = \beta(E)$ is a continuous nondecreasing Lipschitz function in E. Conversely, γ the inverse map of β, is a strictly monotone graph as defined in (2.2).

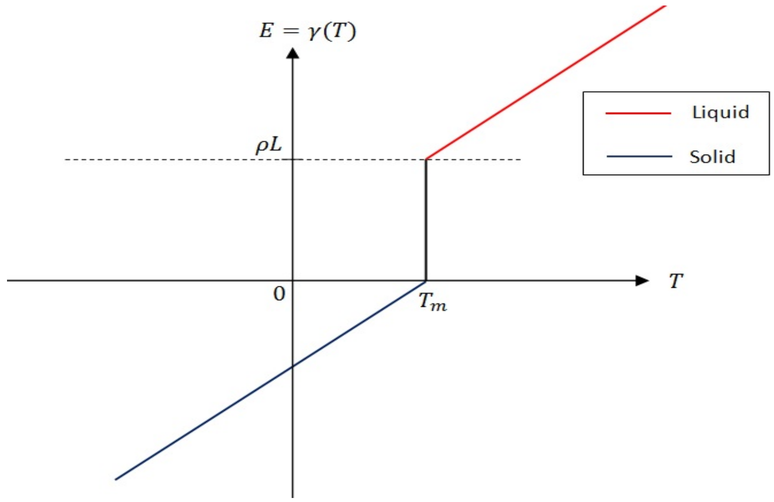

Figure 2.1 The enthalpy set-valued graph $\gamma(T)$

Thus, the equation of enthalpy E can be written as

$$E_t = \nabla \cdot (\kappa \nabla \beta(E)), \qquad \kappa \frac{\partial}{\partial \nu} \beta(E) = g. \tag{2.4}$$

So, if the enthalpy E is given, then the temperature is defined by $\theta = \beta(E)$, and hence the interface is defined by $\{\theta = T_m\}$.

2.2 Strong Form of the Two-Phase Stefan Problem

In this section we discuss the strong differential form of the two-phase Stefan problem. We introduce the moving interface problem based on our enthalpy formulation. First, we define the interface set Γ_t as

$$\Gamma_t = \{x \in \Omega : \theta(t, x) = T_m\}$$

where Γ_t is assumed to be a surface representing the interface between the solid region Ω_t^- where $\theta < T_m$, and the liquid region Ω_t^+ where $\theta > T_m$, with $\Omega_t^- \cap \Omega_t^+ = \Gamma_t$, and Γ_t is the free common boundary (interface) in between the two regions. The solidification temperature at the interface is assumed to be constant and equals T_m.

The standard vector form of the single-phase heat conduction equation is

$$\rho\, c \frac{\partial T}{\partial t} = \kappa\, \Delta T, \tag{2.5}$$

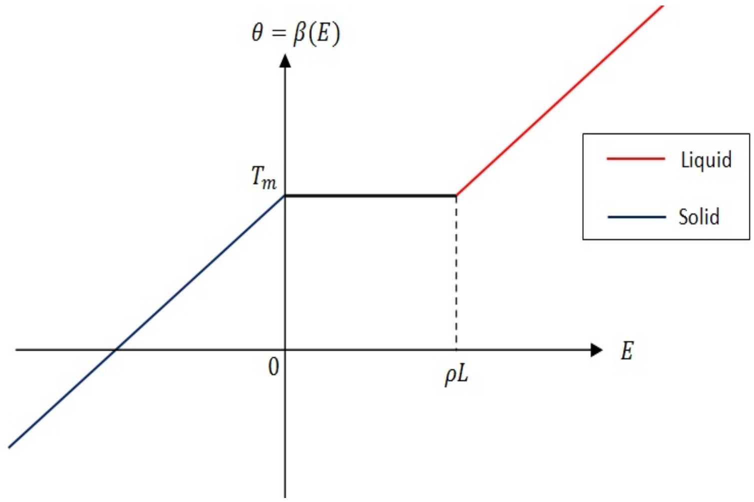

Figure 2.2 The Inverse of Enthalpy Graph $\beta(E)$

where T is the temperature, ρ is the material density, c is the specific heat, and κ is the thermal conductivity of the material. Thus, we have the separate heat conduction for each phase, i.e. liquid and solid phases, as

$$\begin{cases} \rho c_s \dfrac{\partial T_s}{\partial t} = \kappa_s \Delta T_s, \quad \text{for } \ x \in \Omega_t^- \\ \\ \rho c_\ell \dfrac{\partial T_\ell}{\partial t} = \kappa_\ell \Delta T_\ell, \quad \text{for } \ x \in \Omega_t^+. \end{cases}$$

The boundary flux control for (2.5) is given by

$$\kappa \frac{\partial}{\partial \nu} T = g, \tag{2.6}$$

at a portion Γ_c of the exterior boundary $\partial\Omega$, which is the control portion, and otherwise the flux is zero at $\partial\Omega \setminus \Gamma_c$.

We are interested in tracking the motion of the interface $X(t) = \{x \in \Omega : \theta(t,x) = T_m\}$ on Γ_t in the normal direction, i.e.

$$\frac{d}{dt} X(t) = V(t, X(t))\, \nu(t, X(t))$$

where $V(t, X(t))$ is the velocity of the interface motion. By the distribution theory, the latent heat of the system L, is related to the difference of flux as

$$\int_{\Gamma_t} (\rho L \frac{d}{dt} X(t))\ \phi\ ds = \int_{\Gamma_t} [\kappa \frac{\partial T}{\partial \nu}]\ \phi\ ds$$

for all smooth functions ϕ. Thus, we have

$$\rho L\ V(t, X(t)) = [\kappa \frac{\partial T}{\partial \nu}]_{\Gamma_t} = \kappa_\ell \frac{\partial T_\ell}{\partial \nu} - \kappa_s \frac{\partial T_s}{\partial \nu} \tag{2.7}$$

where κ_ℓ, κ_s are conductivity of liquid and solid, respectively. Thus, we have a jump condition, often called Stefan condition, on Γ_t which determines the evolution of the interface motion with velocity $V(t, x(t))$.
In summary, the governing equations for the differential form of Stefan problem are given by

$$\begin{cases} \rho_s c_s \dfrac{\partial T_s}{\partial t} = \kappa_s \Delta T_s, \quad \text{for } x \in \Omega_t^-, \quad T_s = T_m, \quad \text{on } \Gamma_t \\ \\ \rho_\ell c_\ell \dfrac{\partial T_\ell}{\partial t} = \kappa_\ell \Delta T_\ell, \quad \text{for } x \in \Omega_t^+, \quad T_\ell = T_m, \quad \text{on } \Gamma_t \\ \\ \rho L\ V(t, X(t)) = [\kappa \dfrac{\partial T}{\partial \nu}], \quad \text{on } \Gamma_t. \end{cases} \tag{2.8}$$

By the last equation, we compute the flux differences and determine the evolution of the interface. In the system (2.8), the unknown pair is (T, Γ_t), where T is the temperature field and Γ_t is the interface location. Thus, if the interface Γ_t is given, we can determine the temperature at each phase, and control the motion of the free boundary.

2.3 Weak Solution of Enthalpy Formulation

In this section we show the existence of weak solutions to the enthalpy formulation with boundary control. First, we introduce the weak form of enthalpy equation. Then, we establish an apriori bound for enthalpy solutions.
For a fixed domain Ω with $\Gamma_c \subseteq \partial\Omega$, the enthalpy formulation can be written using Green's formulas as

$$\int_\Omega E_t\ \phi\ dx = \int_\Omega (\kappa \Delta \theta)\ \phi\ dx = \int_{\Gamma_c} g\ \phi\ ds - \int_\Omega \kappa \nabla\theta\ \nabla\phi\ dx \tag{2.9}$$

for all test functions $\phi \in H^1(\Omega)$, where we used $\kappa \frac{\partial}{\partial \nu}\theta = g$. The advantage of writing the weak form is that the control g appears explicitly in the weak form (2.9). Equation (2.9) is equivalent to

$$(\kappa\Delta\theta, \phi) = -\kappa(\nabla\theta, \nabla\phi)_\Omega + \kappa(\frac{\partial\theta}{\partial\nu}, \phi)_{\Gamma_c} = -(\kappa\nabla\theta, \nabla\phi)_\Omega + (g, \phi)_{\Gamma_c}. \tag{2.10}$$

We construct the weak solution of (2.9) by considering the difference scheme in time for (2.4)

$$\frac{E^n - E^{n-1}}{\lambda} = \kappa\Delta\beta(E^n), \qquad \kappa\frac{\partial}{\partial\nu}\beta(E^n) = g^n, \tag{2.11}$$

where $\lambda > 0$ is the time step size. Let $\theta^n = \beta(E^n)$, then (2.11) can be written as

$$E^n - E^{n-1} = \tau\Delta\theta^n, \qquad \kappa\frac{\partial}{\partial\nu}\theta^n = g^n, \tag{2.12}$$

where $\tau = \kappa\lambda$. Now, let $j : \mathbb{R} \to \mathbb{R}$ be a strictly convex functional, and its sub-differential $\partial j = \gamma(\cdot)$ is a maximal monotone graph. The functional j can be written as

$$j(\theta) = \begin{cases} \frac{1}{2}\rho c_s\theta^2, & \theta \leq 0, \\ \\ \frac{1}{2}\rho c_\ell\theta^2 + \rho L\theta, & \theta \geq 0, \end{cases} \tag{2.13}$$

where $\theta = T - T_m$. Then, equation (2.12) can be written as

$$\tau\Delta\theta^n + E^{n-1} \in \partial j(\theta^n), \qquad \kappa\frac{\partial\theta^n}{\partial\nu} = g^n, \tag{2.14}$$

since $\partial j = \gamma$ is a set-valued graph. We define the solution of (2.12) by minimizing the cost functional

$$\frac{1}{2}\int_\Omega (\tau|\nabla\theta|^2 + j(\theta) - E^{n-1}(x)\theta) - \lambda(g^n, \theta)_{\Gamma_c}\, dx, \qquad \forall\, \theta \in H^1(\Omega). \tag{2.15}$$

Since the minimizing formula (2.15) is quadratic, then it is coercive and strictly convex in θ. Thus the existence of a unique solution is guaranteed. Indeed, given E^{n-1} and g^n, then the minimizer $\theta \in H^1(\Omega)$ of (2.15), is the unique solution of (2.14), given that $E^n \in L^2(\Omega)$ and $g^n \in L^2(\Gamma_c)$.

2.3.1 An Apriori Bound of the Finite Difference Solution

Now, we establish an apriori bound for the difference scheme solutions in order to be able to pass the limit as $\lambda \to 0$. First, let

$$\Phi(E) = \int_0^E \beta(z)\, dz = T_m E + \begin{cases} \dfrac{1}{2\rho c_s}|E|^2, & E \le 0, \\ 0, & 0 \le E \le \rho L, \\ \dfrac{1}{2\rho c_\ell}|E-\rho L|^2, & E \ge \rho L. \end{cases} \tag{2.16}$$

Then, Φ is convex. Recall the basic inequality for differentiable convex functions

$$f(x) \ge f(\hat{x}) + \nabla f(x)^T (x - \hat{x}), \quad \forall\, \hat{x} \in \text{ dom} f. \tag{2.17}$$

Now, we show the L^2 estimate for $\nabla\theta^n$ and E^n, i.e. $\nabla\theta^n \in L^2(0,T;L^2(\Omega))$ and $E^n \in L^\infty(0,T;L^2(\Omega))$. First, recall equation (2.12)

$$E^n - E^{n-1} = \tau\Delta\theta^n,$$

where

$$\nabla\theta^n = \beta'(E^n)\nabla E^n. \tag{2.18}$$

since $\theta^n = \beta(E^n)$. Also, from equation (2.17) we have

$$\Phi(E^{n-1}) - \Phi(E^n) \ge (\Phi'(E^n), E^{n-1} - E^n)$$

which implies that

$$\Phi(E^{n-1}) - \Phi(E^n) \ge (\beta(E^n), E^{n-1} - E^n). \tag{2.19}$$

Substituting $\theta^n = \beta(E^n)$ in (2.19), we get

$$\Phi(E^{n-1}) - \Phi(E^n) \ge (\theta^n, E^{n-1} - E^n).$$

So, we get

$$(E^n - E^{n-1}, \theta^n) \le \Phi(E^n) - \Phi(E^{n-1}). \tag{2.20}$$

Now, by Green's identities we have

$$(\tau\,\Delta\theta^n, \theta^n) = -\tau|\nabla\theta^n|^2 + \tau(g^n, \theta^n)_{\Gamma_c}.$$

Then, it follows from (2.11) that

$$\int_\Omega \Phi(E^n)\, dx - \int_\Omega \Phi(E^{n-1})\, dx + \tau |\nabla \theta^n|^2 \le \lambda (g^n, \theta^n)_{\Gamma_c}, \tag{2.21}$$

Then, summing (2.21) in time, we obtain

$$\int_\Omega \Phi(E^n)\, dx + \sum_{k=1}^{n} \kappa\lambda |\nabla\theta^n|^2 \le \int_\Omega \Phi(E^0)\, dx + \sum_{k=1}^{n} \lambda |g^n|^2_{L^2(\Gamma)}. \tag{2.22}$$

where $\theta^n = \beta(E^n)$, and $\beta(E^n)$ is Lipschitz.
Note that

$$(\theta^n, g^n) \le |\theta^n|_{H^1(\Omega)} |g^n|_{H^{-1/2}(\Gamma_c)}. \tag{2.23}$$

Estimating $|\nabla\theta^n|$ in (2.22) is not enough for the full H^1-norm, since the full norm of θ^n in $H^1(\Omega)$ is given by

$$|\theta^n(t)|^2_{H^1(\Omega)} = (\theta^n, \theta^n) + (\nabla\theta^n, \nabla\theta^n).$$

Now, we have the L^2 bound for θ^n is given by

$$|\theta^n(t)|_{L^2(\Omega)} \le C_0 |E^n|^2 \le C_1 \Phi(E^n) + C_2. \tag{2.24}$$

Thus, there exists some constant $C > 1$ such that

$$\int_\Omega \Phi(E^n)\, dx + \frac{1}{2}\sum_{k=1}^{n} \kappa\lambda |\beta'(E^n)\nabla E^n|^2 \le \int_\Omega \Phi(E^0)\, dx + C\sum_{k=1}^{n} \lambda |g^n|^2_{L^2(\Gamma)}. \tag{2.25}$$

Also, we have the L^1 bound of E^n as follows. In fact, from (2.11), we have

$$(E^n - E^{n-1}, \rho_\varepsilon(\theta^n) = \int_\Omega \Delta\theta^n \ \rho_\varepsilon(\theta^n)\, dx = \int_\Gamma \frac{\partial\theta^n}{\partial\nu}\ \rho_\varepsilon(\theta^n)\, ds - \int_\Omega |\nabla\theta^n|^2 \ \rho'_\varepsilon(\theta^n)\, dx$$

So,

$$\int_\Omega |E^n| - \int_\Omega |E^{n-1}| \le \lambda \int_{\Gamma_c} |g^n|\, ds \tag{2.26}$$

Therefore, we get

$$\int_\Omega |E^n|\, dx - \int_\Omega |E^0|\, dx \le \lambda \sum_{k=0}^{n} \int_{\Gamma_c} g^k\, ds = M_0,$$

which implies that

$$\int_\Omega |E^n|\, dx \leq M, \tag{2.27}$$

and then, we obtain the following estimate

$$\int_\Omega \theta^n\, dx = \int_\Omega \beta(E^n)\, dx \leq L \int_\Omega |E^n|\, dx \leq LM. \tag{2.28}$$

where L is the Lipschitz constant of $\beta(E^n)$. This estimate completes the full norm in H^1 and it is enough for us to be able to pass the limit as $\lambda \to 0$.

2.4 Convergence of Weak Solutions

In this section we show the existence of weak solution of enthalpy formulation (2.9) by passing the limit as $\lambda \to 0$ using Aubin's lemma. First, we discuss the statement of Aubin's lemma. Then, we apply Aubin's lemma to pass the limit in (2.11) and prove the existence of weak solutions.

2.4.1 Aubin's Lemma

Aubin's lemma is an important result in Sobolev spaces theory. The theorem gives a criterion for the compact embedding in $L^2(0,T;X)$. The Lemma is useful in the study of nonlinear evolution equations. In particular, it helps us to prove the existence of approximate solutions constructed using Galerkin method. The statement of Aubin's lemma is given as follows.

Aubin's Lemma:
Let X_0, X and X_1 be Banach spaces with $X_0 \subseteq X \subseteq X_1$ and X_0 is compactly embedded in the pivoting space X and X is continuously embedded in X_1. Assume that X_0 and X_1 are reflexive. Then

$$W := \{u \in L^2(0,T;X_0) : u_t \in L^2(0,T;X_1)\}$$

is compactly embedded into $L^2(0,T;X)$.

The proof of Aubin's lemma is discussed in [7, 72]. The original proof of the lemma by Aubin [7] requires the spaces X_0 and X_1 in the statement of the lemma to be reflexive, but Simon [60] proved the result without this assumption.

2.4.2 Passing the Limit as $\lambda \to 0$ Using Aubin's Lemma

Recall equation (2.4) which can be written as

$$E_t = \kappa \Delta \theta, \qquad \kappa \frac{\partial \theta}{\partial \nu} = g, \tag{2.29}$$

and recall from last section that

$$\theta^n \in L^2\big(0, T; H^1(\Omega)\big), \quad \text{and} \quad \nabla \theta^n \in L^2\big(0, T; L^2(\Omega)\big).$$

In order to be able to use Aubin's lemma, we need to show that

$$E^n \in L^2\big(0, T; H^1(\Omega)\big), \quad \text{and} \quad \frac{dE^n}{dt} \in L^2\big(0, T; H^1(\Omega)^*\big).$$

To show that

$$\frac{dE^n}{dt} \in L^2\big(0, T; H^1(\Omega)^*\big), \tag{2.30}$$

recall the weak form (2.10)

$$(\kappa \nabla \theta, \nabla \phi)_\Omega - (g, \phi)_{\partial \Omega} = \big(\frac{dE}{dt}, \phi\big), \quad \forall \, \phi \in H^1(\Omega), \tag{2.31}$$

so, we have

$$|(\kappa \nabla \theta, \nabla \phi)_\Omega - (g, \phi)_{\partial \Omega}| \le \alpha(t) \; |\phi|_{H^1}$$

where

$$\alpha(t) = \kappa |\nabla \theta(t)| + |g(t)|_{H^{-1/2(\Gamma)}} \; \in L^2(0 : T).$$

Thus, we can conclude that (2.30) holds. Next, to show that

$$E^n \in L^2\big(0, T; H^1(\Omega)\big),$$

recall equation (2.18)

$$\nabla \theta = \beta'(E) \nabla E$$

which can be written as

$$\nabla E = \beta'(E)^{-1} \, \nabla \theta,$$

thus, without loss of generality, we get

$$\int_0^T |\nabla E^n|_{L^2} \leq M,$$

and then we can conclude that

$$E^n \in L^2\big(0, T; H^1(\Omega)\big).$$

So, we have

$$\begin{cases} E^n \xrightarrow{w} E, \quad \text{in } \; L^2\big(0, T; H^1(\Omega)\big), \\ \\ E^n \xrightarrow{s} E, \quad \text{in } \; L^2\big(0, T; L^2(\Omega)\big). \end{cases} \tag{2.32}$$

Next, consider the piece-wise linear functional

$$E^n(t) = E^{n-1} + \big(\frac{E^n - E^{n-1}}{\lambda}\big)(t - t_n), \tag{2.33}$$

where $t_n - t_{n-1} = \lambda$. The time derivative of (2.33) is

$$\frac{dE^n}{dt} = \frac{E^n - E^{n-1}}{\lambda}. \tag{2.34}$$

Consider the weak form of (2.34), given by

$$\big(\frac{E^n - E^{n-1}}{\lambda}, \phi\big) = \kappa(\nabla \beta(\widetilde{E^n}(t)), \nabla \phi)_\Omega - (g, \phi)_{\partial\Omega}, \tag{2.35}$$

where we used equation (2.31), and

$$\widetilde{E^n}(t) = E^n, \quad \text{on } \; [t_{n-1}, t_n].$$

Now, we show that

$$|\widetilde{E^n}(t) - E^n(t)|_{L^2} \leq M \; \lambda^2. \tag{2.36}$$

since

$$|\widetilde{E^n}(t) - E^n(t)| = |E^n - \big(E^n - (t - t_n)\frac{E^n - E^{n-1}}{\lambda}\big)|.$$

Multiply equation (2.35) against E^n, we have

$$\big(\frac{E^n - E^{n-1}}{\lambda}, E^n\big) = \kappa(\beta'(E^n) \, \nabla E^n, \nabla E^n) - (g, E^n). \tag{2.37}$$

Completing the square in equation (2.37), we get

$$\frac{\frac{1}{2}|E^n|^2 - \frac{1}{2}|E^{n-1}|^2 + \frac{1}{2}|E^n - E^{n-1}|^2}{\lambda} = \kappa(\beta'(E^n)\,\nabla E^n, \nabla E^n) - (g, E^n) \leq -(g, E^n)_{\partial\Omega},$$

since $(\beta'(E^n)\,\nabla E^n, \nabla E^n)$ is positive. Now, summing over n, we get

$$\frac{1}{2}|E^m|^2 + \sum_{n=1}^{m} \frac{E^n - E^{n-1}}{\lambda} \leq \frac{1}{2}|E^0|^2 + M.$$

So, we get

$$\int_{t_{n-1}}^{t_n} \left|(t - t_n)^2 \,\big(\frac{E^n - E^{n-1}}{\lambda}\big)\right|^2 \leq M\,\lambda^2,$$

which implies that equation (2.36) is satisfied. So

$$\widetilde{E^n} \xrightarrow{s} E$$

Thus, we have

$$E^n \xrightarrow{s} E, \quad \text{in } \; L^2\big(0, T; L^2(\Omega)\big).$$

Next, since β is Lipschitz, we have

$$|\beta(E_1) - \beta(E_2)| \leq L|E_1 - E_2|,$$

so, we have

$$\beta(E^n) \xrightarrow{s} \beta(E), \quad \text{in } \; L^2\big(0, T; L^2(\Omega)\big). \tag{2.38}$$

where, using Green's formula, we have $\forall\phi \in \{\phi \in H^1(\Omega) : \Delta\phi \in L^2(\Omega), n \cdot \nabla\phi = 0\} \subseteq H^2(\Omega)$, which is dense in $H^1(\Omega)$,

$$(\nabla\beta(E^n), \nabla\phi) = \int_{\partial\Omega} (n \cdot \nabla\phi)\beta(E^n)\; ds - \int_{\Omega} \beta(E^n)\;\Delta\phi\; dx.$$

Thus, from (2.38), $E^n \to E$ is a weak solution to the enthalpy equation (2.9).

2.5 Lipschitz Continuity of Solution E with Respect to Control g

In this section we prove the smoothness of the enthalpy solution. We show that the enthalpy solution E is Lipschitz continuous with respect to control g. We also conclude that $E(g)$ has a unique solution. First, consider the difference scheme in time

$$\begin{cases} \dfrac{E^n - E^{n-1}}{\lambda} = \kappa\Delta\theta, \quad \kappa\dfrac{\partial\theta}{\partial\nu} = g, \\ \\ \dfrac{\hat{E}^n - \hat{E}^{n-1}}{\lambda} = \kappa\Delta\hat{\theta}, \quad \kappa\dfrac{\partial\hat{\theta}}{\partial\nu} = \hat{g}. \end{cases} \tag{2.39}$$

Adding up the two equations in (2.39)

$$\frac{\delta E^n - \delta E^{n-1}}{\lambda} = \kappa\Delta\delta\theta, \quad \kappa\frac{\partial}{\partial\nu}\delta\theta = \delta g, \tag{2.40}$$

where $\delta E = E - \hat{E}$ and $\delta g = g - \hat{g}$. Let

$$\operatorname{sign}_\epsilon(\delta E^n) = \operatorname{sign}_\epsilon(\delta\theta^n),$$

then using Green's formula, we have

$$(\kappa\Delta\delta\theta^n, \operatorname{sign}_\epsilon(\delta\theta^n)) = -\kappa(\nabla\delta\theta^n \operatorname{sign}'_\epsilon(\delta\theta^n), \nabla\delta\theta^n) - (\delta g, \operatorname{sign}_\epsilon(\delta\theta^n)) \geq -(\delta g, \operatorname{sign}_\epsilon(\delta\theta^n)), \tag{2.41}$$

since $(\nabla\delta\theta^n \operatorname{sign}'_\epsilon(\delta\theta^n), \nabla\delta\theta^n) \geq 0$. Thus, from equations (2.40) and (2.41) we get

$$(\frac{\delta E^n - \delta E^{n-1}}{\lambda}, \operatorname{sign}_\epsilon(\delta\theta^n)) \leq -(\delta g, \operatorname{sign}_\epsilon(\delta\theta^n)). \tag{2.42}$$

Taking the limit as $\epsilon \to 0$ in equation (2.42), we get

$$\frac{|\delta E^n|_1 - |\delta E^{n-1}|_1}{\lambda} \leq \int_{\Gamma_c} |\delta g| \, ds, \tag{2.43}$$

which implies that

$$|\delta E^n(T)|_1 \leq \int_0^T \int_{\Gamma_c} |\delta g| \, ds \, dt, \tag{2.44}$$

where we used $|\delta E^n(0)| = 0$.

Another way to show the continuity of E with respect to control g is given as follows. Apply the inverse of Laplacian operator to equation (2.40)

$$\begin{cases} (-\Delta)^{-1}(\delta E^n - \delta E^{n-1}) = \kappa \delta\theta^n + \xi, \\ \\ -\Delta\xi = 0, \quad \kappa \dfrac{\partial \xi}{\partial \nu} = g, \end{cases} \tag{2.45}$$

where g is extended to $L^2(\Omega)$.

Testing equation (2.45) against δE^n and using that $\theta^n = \beta(E^n)$, we get

$$((-\Delta)^{-1}(\delta E^n - \delta E^{n-1}), \delta E^n) = \kappa(\beta(E^n) - \beta(E^{n-1})), \delta E^n) + (\xi, (-\Delta)^{-1}\delta E^n). \tag{2.46}$$

Thus, we get

$$\frac{1}{2}(|\delta E^n|^2_{V^*} - |\delta E^{n-1}|^2_{V^*} + |\delta E^n - \delta E^{n-1}|^2_{V^*}) \leq (\xi, (-\Delta)^{-1}\delta E^n) \leq |g|_{H^{-1/2}(\Gamma)}\, |\delta E^n|_{V^*}, \tag{2.47}$$

where $V = H^1(\Omega)$, and $V^* = H^1(\Omega)^*$. So, we get the following estimate

$$|\delta E^n(T)|_{V^*} \leq M \int_0^T |\delta g|_{H^{-1/2}(\Gamma)}\, dt, \tag{2.48}$$

where we used $|\delta E^n(0)| = 0$.

Chapter 3

Optimal Control Problem for the Motion of the Interface of Stefan Problem

In this chapter we consider the optimal control formulation for enthalpy by the boundary control g. Consider the optimal control problem of tracking type of the form

$$\min \ J(E,g) = \frac{1}{2}\int_0^T |E-\bar{E}|^2_{L^2(\Omega)}\, dt + \frac{\gamma}{2}|E(T)-\bar{E}|^2_{L^2(\Omega)} + \frac{\alpha}{2}\int_0^T |g|^2_{L^2(\Gamma_c)}\, dt, \tag{3.1}$$

subject to the control constraint $|g| \leq \delta$ and (2.4), where $\bar{E}$ is the desired enthalpy state, $|E(T)-\bar{E}|^2$ is the terminal cost, and $\alpha > 0$, $\gamma > 0$, $\delta > 0$ are properly chosen.
Alternatively, the cost functional for the enthalpy can be written using the level set formulation. To see that, let $\bar{\Gamma}_t$ be the desired motion of the interface and let $\phi(t,x)$ be a distance function to the desired interface $\bar{\Gamma}_t$, i.e. $\phi = \text{dist}(x, \bar{\Gamma}_t)$, and the zero level set $\bar{\Gamma}_t = \{x \in \Omega : \phi(t,x) = 0\}$ where the optimal control problem is given by

$$\min \ J(E,g) = \frac{1}{2}\int_0^T |\phi(\beta(E(t)))|^2\, dt + \frac{\alpha}{2}\int_0^T |g|^2_{\Gamma_c}\, dt. \tag{3.2}$$

Also, we can choose the cost functional for the enthalpy in terms of the temperature θ as

$$\min \ J(E,g) = \frac{1}{2}\int_\Gamma |\theta(x,t)|^2\, ds_x + \frac{\alpha}{2}\int_0^T |g|^2_{\Gamma_c}\, dt. \tag{3.3}$$

In summary, we consider the control cost functional

$$\min \; J(E,g) = \int_\Omega \Psi(E)\, dx + \gamma\, \Psi\big(E(T)\big) + \frac{\alpha}{2}\int_0^T |g|^2_{\Gamma_c}\, dt, \tag{3.4}$$

where Ψ represents the cost functionals given above. We will first establish the existence of optimal control for (3.1). Then, we will use Lagrange Calculus to obtain the necessary optimality conditions.

3.1 Existence of Optimal Control

In this section we establish the existence of optimal control for (3.1). From the weak solution that we have established in the previous chapter, the enthalpy E can be written as a function of g, i.e. $E = E(g)$. So, let $\tilde{J}(g)$ be the composite function $\tilde{J}(g) = J(E(g), g)$. Then, the functional $\tilde{J}(g)$ is coercive, i.e.

$$\tilde{J}(g) \to \infty \text{ as } |g|_{L^2(\Gamma_c)} \to \infty, \qquad \text{with } \alpha > 0,$$

and weakly lower semi-continuous, i.e.

$$\lim_{n\to\infty} \inf \tilde{J}(g^n) \geq \tilde{J}(g), \;\text{ assuming }\; g^n \overset{w}{\rightharpoonup} g, \;\text{ in } L^2(\Gamma_c),$$

if we prove the weak continuity of the equality constraint, i.e. if (E^n, g^n) converges weakly to (E, g), then (E, g) satisfies equation (2.4), i.e.

$$E_t = \nabla \cdot (\kappa \nabla \beta(E)), \qquad \kappa \frac{\partial}{\partial \nu}\beta(E) = g,$$

then the existence of optimal control is guaranteed. In fact, the weak continuity of the equality constraint follows from the following weak form

$$(\beta(E^n), \Delta\phi) + (g^n, \phi)_{\Gamma_c} = 0, \quad \forall\, \phi \in L^2(0,T; H^2(\Omega)), \;\text{ satisfying }\; \frac{\partial \phi}{\partial \nu} = 0.$$

Since E^n converges strongly to E in $L^2\big(0,T; L^2(\Omega)\big)$ as we argued in equation (2.32) in section (2.4.2), then we conclude that (E, g) satisfies (2.4). So, we have the weak continuity of the equality constraint. Thus, by Weierstrass theorem discussed in Appendix A, there exists a minimizer $g^* \in L^2(\Gamma_c)$ to the problem (3.1).

3.2 Lagrangian Functional and Adjoint Equation

Define the Lagrangian functional as

$$\mathcal{L}(E,g,p) = J(E,g) + \int_0^T (\kappa\Delta\beta(E) - \frac{dE}{dt}, p)\, dt. \tag{3.5}$$

By the integration by parts and Green's formula we have

$$\mathcal{L}(E,g,p) = J(E,g) + \int_0^T \big(-\kappa(\nabla\beta(E),\nabla p) + (g,p)_{\Gamma_c} + (\frac{dp}{dt},E)\big)\, dt - (E(T),p(T)) + (E(0),p(0)),$$

where we used $\kappa\frac{\partial}{\partial\nu}\beta(E) = g$. The Gateaux derivative of $\mathcal{L}$ with respect to E is given by

$$\mathcal{L}_E(E,g,p)(h) = \int_0^T (\Psi'(E),h) + (\kappa\nabla\beta'(E)\,\Delta p + \frac{dp}{dt},h)\, dt + (h(T),p(T) - \gamma\,\Psi'(E(T))),$$

for all directions h satisfying $h(0) = 0$. Hence, we have the adjoint equation for p as

$$-\frac{dp}{dt} = \kappa\,\beta'(E)\,\Delta p + \Psi'(E), \quad p(T) = \gamma\,\Psi'(E(T)) \text{ and } \frac{\partial p}{\partial\nu} = 0. \tag{3.6}$$

We next show that the adjoint equation (3.6) has a solution p.

3.2.1 Existence of the Adjoint State p

To show that the adjoint equation (3.6) has a solution, consider the backward in time discretization of (3.6), i.e. given p^n, we have

$$-\frac{p^n - p^{n-1}}{\Delta t} = \kappa\beta_\varepsilon'(E^n)\,\Delta p^{n-1} + \Psi'(E^n), \qquad \frac{\partial}{\partial\nu}p^{n-1} = 0 \tag{3.7}$$

where $\beta_\varepsilon \in C^1(\mathbb{R})$ is a regularization of β defined by

$$\beta_\varepsilon(s) = \frac{1}{2\varepsilon}\int_{s-\varepsilon}^{s+\varepsilon} \beta(z)\, dz \tag{3.8}$$

$\beta_\varepsilon'(E) \geq \varepsilon$ for some arbitrary $\varepsilon > 0$, and with terminal condition $p^N = \gamma\,\Psi'(E^N)$. Then, equation (3.7) can be written as

$$-\Delta p^{n-1} = -\frac{p^{n-1} - p^n}{\kappa\Delta t\;\beta_\varepsilon'(E^n)} + \frac{\Psi'(E^n)}{\kappa\beta_\varepsilon'(E^n)}.$$

Define the bilinear form $a(\cdot,\cdot)$ as

$$a(p,\phi) = (-\Delta p^{n-1},\phi) - \left(\frac{p^{n-1}-p^n}{\kappa\Delta t\ \beta_\varepsilon'(E^n)},\phi\right) + \left(\frac{\Psi'(E^n)}{\kappa\beta_\varepsilon'(E^n)},\phi\right). \tag{3.9}$$

Using Green's formula, the bilinear form can be written as

$$a(p,\phi) = (\nabla p^{n-1},\nabla\phi) - \left(\frac{p^{n-1}-p^n}{\kappa\Delta t\ \beta_\varepsilon'(E^n)},\phi\right) + \left(\frac{\Psi'(E^n)}{\kappa\beta_\varepsilon'(E^n)},\phi\right).$$

The bilinear form $a(\cdot,\cdot)$ is bounded and coercive, thus using Lax-Milgram theorem with $X = H^1(\Omega)$ we conclude that there exists a unique solution p^{n-1}, given p^n and E^n. Hence, we only need to establish an apriori bound for the adjoint solution and then pass the limit as $n\to\infty$.

3.2.2 An Apriori Bound for Solution of Adjoint Equation

To find a priori bound for the adjoint equation (3.6), test equation (3.7) against Δp^{n-1}

$$(-\frac{p^n-p^{n-1}}{\Delta t},\Delta p^{n-1}) = (\beta_\varepsilon'(E^n)\ \Delta p^{n-1},\Delta p^{n-1}) + (\Psi'(E^n),\Delta p^{n-1})$$

then, using Green's formula we have

$$(\frac{\nabla p^{n-1}}{\Delta t},\nabla p^{n-1}) + (\beta_\varepsilon'(E^n)\ \Delta p^{n-1},\Delta p^{n-1}) = -(\frac{\nabla p^n}{\Delta t},\nabla p^{n-1}) + (\Psi'(E^n),\Delta p^{n-1}).$$

Summing in n, multiplying by Δt, and completing the square, we get

$$(\nabla p^n,\nabla p^n) + \sum_n \frac{\Delta t}{2}(\beta_\varepsilon'(E^n)\ \Delta p^{n-1},\Delta p^{n-1}) = -(\nabla p^N,\nabla p^N) + \sum_n \frac{\Delta t}{2\varepsilon}(\Psi'(E^n),\Delta p^{n-1}).$$

Now, the sum can be bounded by

$$\frac{1}{2}(\beta_\varepsilon'(E^n)\ \Delta p^{n-1},\Delta p^{n-1}) + \frac{1}{2\varepsilon}(\Psi'(E^n),\Delta p^{n-1}) \le \frac{1}{2}(\beta_\varepsilon'(E^n)\ \Delta p^{n-1},\Delta p^{n-1}) + \frac{1}{2\varepsilon}|\Psi'(E^n)|_{L^2(\Omega)}$$

Letting $\Delta t\to 0$, we have $p^n\to p$ and $p\in H^1(0,T;L^2(\Omega))\cap L^2(0,T;H^2(\Omega))$, with

$$\int_t^T (\beta_\varepsilon'(E)\ \Delta p,\Delta p)\ dt + |\nabla p|^2_{L^2(\Omega)} \le \frac{1}{2\varepsilon}\int_t^T |\Psi'(E)|^2.$$

As we mentioned above, this argument is valid only if $\beta' \ge \varepsilon$.

3.3 Necessary Optimality Condition

In this section we use Lagrange calculus to obtain the adjoint equation and necessary optimality. The details of the general case are discussed in Appendix B. Recall the Lagrange functional introduced in section (3.2) for the enthalpy constraint (2.4)

$$\mathcal{L}(E,g,p) = J(E,g) + \int_0^T \big(-\kappa(\nabla\beta(E),\nabla p) + (g,p)_{\Gamma_c} - (\frac{dE}{dt},p)\big)\,dt. \tag{3.10}$$

In this case the optimality condition for g^* is given by

$$\mathcal{L}_g(E,g,p) = \alpha g^* + p = 0, \text{ at } \Gamma_c, \tag{3.11}$$

where p satisfies the adjoint equation (3.6), i.e.

$$-\frac{dp}{dt} = \kappa\,\beta'(E)\,\Delta p + \Psi'(E), \quad \frac{\partial p}{\partial\nu} = 0, \quad p(T) = \gamma\,\Psi'(E(T)).$$

The condition (B.8) in Appendix B, holds since $g \to E(g)$ is Lipschitz continuous as shown in section(2.5).

In summary, the necessary optimality with the adjoint system can be written as the following two points boundary value problem for (E,p)

$$\begin{cases} E_t = \kappa\Delta\beta(E), \quad \kappa\dfrac{\partial}{\partial\nu}\beta(E) = g, \\[2ex] -\dfrac{dp}{dt} = \kappa\,\beta'(E)\,\Delta p + \Psi'(E), \quad \dfrac{\partial p}{\partial\nu} = 0, \\[2ex] \alpha g^* + p = 0, \\[2ex] E(0,x) = E_0, \quad \text{and} \quad p(T,x) = \gamma\,\Psi'(E(T)). \end{cases} \tag{3.12}$$

3.4 Numerical Methods for Enthalpy Formulation of the Controlled Tow-Phase Stefan Problem

Recall the time discretization scheme of enthalpy (2.12)

$$E^n - E^{n-1} = \tau\Delta\theta^n, \quad \kappa\frac{\partial}{\partial\nu}\theta^n = g^n, \quad \theta^n = \beta(E^n), \tag{3.13}$$

where $\beta(E)$ is the continuous nondecreasing Lipschitz function in E given by (2.3), i.e.

$$\beta(E) = \begin{cases} T_m + \dfrac{1}{\rho c_\ell}(E - \rho L), & E \geq \rho L, \\ T_m, & 0 \leq E \leq \rho L, \\ T_m + \dfrac{1}{\rho c_s} E, & E \leq 0. \end{cases} \tag{3.14}$$

Also, recall the variational formulation of (3.13), given by minimizing the following cost functional

$$\frac{1}{2}\int_\Omega (\tau|\nabla\theta|^2 + j(\theta) - E^{n-1}(x)\theta) - \lambda(g^n, \theta)_\Gamma \, dx, \qquad \forall\, \theta \in H^1(\Omega), \tag{3.15}$$

i.e. the unique minimizer of (3.13) satisfies (3.15). Our approach is to represent the gradient of the temperature field $|\nabla\theta|^2$ on a lattice. As shown in Figure (3.1), the value of the temperature $\theta = \theta_{ij}$ is at the center of the cell. The discrete form of the gradient of temperature field $|\nabla\theta|^2$ on a lattice is written as

$$\int_\Omega |\nabla_h\theta|^2 \, dx = \frac{1}{2}\sum_{i,j}\frac{1}{2}|\theta_{i,j+1}-\theta_{i,j}|^2+\frac{1}{2}|\theta_{i+1,j+1}-\theta_{i+1,j}|^2+\frac{1}{2}|\theta_{i+1,j}-\theta_{i,j}|^2+\frac{1}{2}|\theta_{i+1,j+1}-\theta_{i,j+1}|^2, \tag{3.16}$$

where we used the trapezoidal rule for the integration over Ω and

$$(g^n, \theta)_\Gamma = \sum_j \theta_{1,j}\; g_{1,j} + \sum_j \theta_{N,j}\; g_{N,j} + \sum_i \theta_{i,1}\; g_{i,1} + \sum_i \theta_{i,N}\; g_{i,N} \tag{3.17}$$

and $g = (g_{1,j}, g_{N,j}, g_{i,1}, g_{i,N})$ on Γ_c.
Thus, the corresponding discrete form of (3.15) in lattice formulation is given as

$$\frac{1}{2}\lambda\kappa(\theta, H\theta) + \sum_{i,j} j(\theta) - (E^{n-1}, \theta)_\Omega - \lambda(g^n, \theta)_\Gamma, \tag{3.18}$$

where H is the Riesz-Representation form of the one dimensional negative Laplacian $-\Delta_h$ given by

$$\int_\Omega |\nabla\theta|^2 \, dx = (H\theta, \theta), \tag{3.19}$$

and

$$H = h \otimes I + I \otimes h. \tag{3.20}$$

The matrix h is the tri-diagonal central difference matrix representing the second derivatives, given by

$$
h = \begin{pmatrix} 1 & -1 & 0 & \dots & 0 & 0 \\ -1 & 2 & -1 & 0 & \dots & 0 \\ 0 & \ddots & \ddots & \ddots & \dots & 0 \\ \vdots & \ddots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & -1 & 2 & -1 \\ 0 & \dots & \dots & 0 & -1 & 1 \end{pmatrix}.
$$

In summary, the equation of enthalpy on a lattice is written as

$$
\frac{E^n - E^{n-1}}{\lambda} = -\kappa H \beta(E^n) + Bg^n, \tag{3.21}
$$

where $(Bg^n, \theta) = (g, \theta)_\Gamma$. Equation (3.21), is an equation for E^n, given E^{n-1} and g^n. It is nonlinear, since $\beta(E)$ is nonlinear. The function $\beta(E)$ is not C^1, but semi-smooth. Thus, we use the well-known Semi-smooth Newton method [47, 49] to solve equation (3.21) for E^n with the Newton derivative of $\beta(E)$, also see Appendix D.1. So, using the tangent equation

$$
\beta(E^+) \sim \beta'(E)(E^+ - E) + \beta(E) \tag{3.22}
$$

where

$$
\beta'(E) = \begin{cases} \dfrac{1}{\rho c_\ell} E, & E > \rho L, \\[2ex] \dfrac{1}{\rho c_s} E, & E \leq \rho L, \end{cases} \tag{3.23}
$$

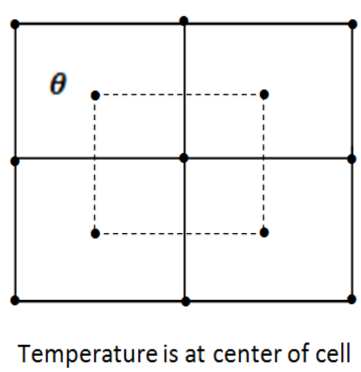

Figure 3.1 The value of the temperature is at the center of the cell

we obtain the linearization as discrete time iterative algorithm for E^n

$$\frac{E_k - E^{n-1}}{\Delta t} = -\kappa\, H(\beta'(E_{k-1})(E_k - E_{k-1}) + \beta(E_{k-1})) + Bg^n, \quad E_0 = E^{n-1}, \tag{3.24}$$

where E_k is the k-th iterate. Equation (3.24) is a linear equation for E_k, and we can show that $E_k \to E^n$.

To write a code for solving E^n, let $q = (\rho c_\ell, \rho c_s)$ be the slopes, then

$$q(E^n - E^{n-1}) = -\kappa H E^n.$$

So, we have

$$\frac{\gamma^{n+1} - \gamma^n}{\Delta t} = -\kappa\, E^{n+1} - g. \tag{3.25}$$

Also, we can write

$$\frac{\gamma^{n+1} - \gamma^n}{\Delta t} = \frac{q(E^{n+1} - E^n)}{\Delta t} \tag{3.26}$$

Thus, from (3.25) and (3.26), we get

$$\frac{q(E^{n+1} - E^n)}{\Delta t} = -\kappa\,(E^{n+1} - E^n) - \kappa\, E^n - g, \tag{3.27}$$

which can be written as

$$(q + \Delta t\, \kappa)(E^{n+1} - E^n) = (-\kappa\, E^n - g)\, \Delta t \tag{3.28}$$

Solving equation (3.28) for E^{n+1}, we get the iterative algorithm

$$E^{n+1} = E^n - (q + \Delta t\, \kappa)^{-1}(\kappa\, E^n + g)\, \Delta t \tag{3.29}$$

The following is the MATLAB code performing the algorithm discussed above.

```
for kkk=1:200; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS; q(j)=rho*cS; q=spdiags(q(:),0,n^2,n^2);
E=E-q*((q+(kS*dt/2)*h)\(kS*dt*h*T0-dt*g0(:))); end
```

3.4.1 Numerical Test Examples

In this section we test the proposed numerical methods for the enthalpy formulation (3.29). The control boundary Γ_c is given as in Figure 3.2. We first test the algorithm for a forward

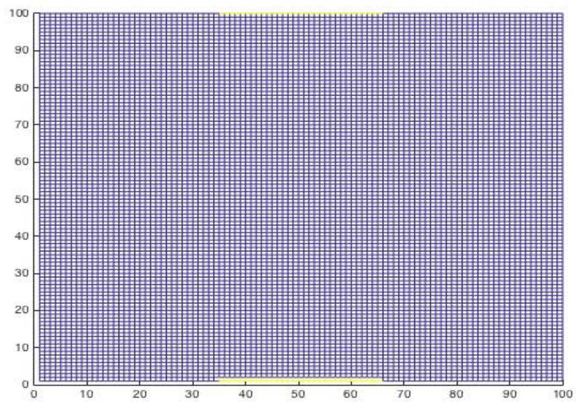

Figure 3.2 The control boundary Γ_c

simulation. We take a constant control $g = 5$ at Γ_c and after $T = 10$ we obtain the splitting of solid region (blue), depicted in Figure 1.2 in Chapter 1. Time snap-shots of the enthalpy function toward the splitting are shown in Figure 3.3 below. We use

```
n=100, rho=1.460; dt=.1;
Tm=32; Ts=25; Tl=90;
L=251.21;
cL=3.31; cS=1.76; kL=.59e-3;  kS=2.16e-3; rhoL=rho*L.
```

Next, we present a numerical test for the optimal control problem. The formulation of our numerical test is to achieve the target state, that is the final state at $T = 1$ of the full horizon problem by the optimal control casted on the half horizon $[0, T/2]$.

First, Figure 3.4 shows the target state. We use the sequential programming method, described in Appendix D.2, and each subproblem of the sequential linearized control problem is solved by the conjugate gradient method, introduced in Appendix D.3. The result of this test is shown in Figure 3.5.

Figure 3.6 shows the resultant optimal feedback flux control on $\Gamma_c \times [0, T/2]$. The values of

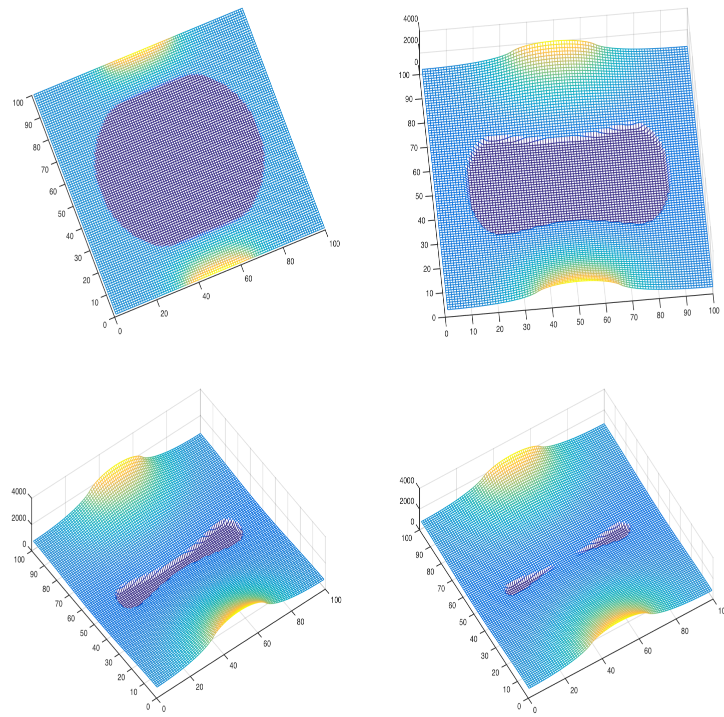

Figure 3.3 Splitting of solid region (blue) by boundary flux

the optimal control on $\Gamma_c \times [0, T/2]$ show that the geometry is symmetric. Thus, control is symmetric in the upper and lower portions of Γ_c. Also, numerical calculations show that the average heat budget over the half horizon is 4.989 compared to 5 over the full horizon. The MATLAB code for the forward problem and the optimal control problem are given as

```
rho=1460; rho=rho/1000; dt=.1;
Tm=32; Ts=25; Tl=90;
L=251.21;
cL=3.31; cS=1.76; kL=.59e-3;  kS=2.16e-3; rhoL=rho*L;

n=100; m=n-1; e=ones(n,1); h=spdiags([-e 2*e -e],[-1:1],n,n);
h(1,1)=1; h(n,n)=1; h=n^2*h; a=1:n*m; a=a(:);
h=kron(speye(n),h)+kron(h,speye(n));
dx=1/n; [x,y]=meshgrid(dx/2:dx:1-dx/2);
phi=(x-.5).^2+(y-.5).^2-.1111; k=find(phi<0); psi(k)=1;
```

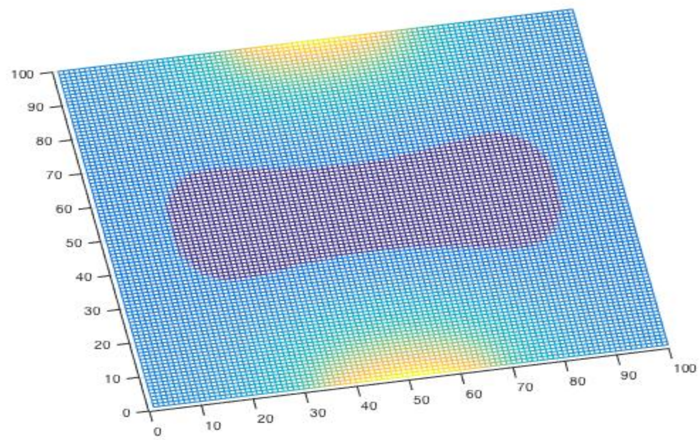

Figure 3.4 The full horizon target state

```
T=33*ones(n,n); T(k)=25; T=(speye(n^2)+1.e-3*h)\T(:);
i=find(T(:)>=Tm); E(i)=rho*cL*(T(i)-Tm)+rhoL;
j=find(T(:)<Tm); E(j)=rho*cS*(T(j)-Tm); E=E(:);
g0=zeros(100); g0(1,35:65)=5; g0(end,35:65)=5; g0=n*g0; E0=E;
Q=speye(n^2); u=ones(1,50); QQ=zeros(n^2,20);

for kkk=1:200; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS; q(j)=rho*cS; q=spdiags(q(:),0,n^2,n^2);
E=E-q*((q+(kS*dt)*h)\(kS*dt*h*T0-dt*g0(:))); end
```

```
E=E0; u=ones(1,50); %we must specify control u=g_{kkk} to compute E
for kkk=1:50; EE(:,kkk)=E;  %%%% we must specify control u=g_{kkk}
for k=1:20; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS; q(j)=rho*cS; q=spdiags(q(:),0,n^2,n^2);
%%%%% Store the solid index jj=[jj j]; (be careful since j has different length)
E=E-q*((q+(kS*dt)*h)\(kS*dt*h*T0-dt*u(kkk)*g0(:))) ; end; end; Eb=E;
```

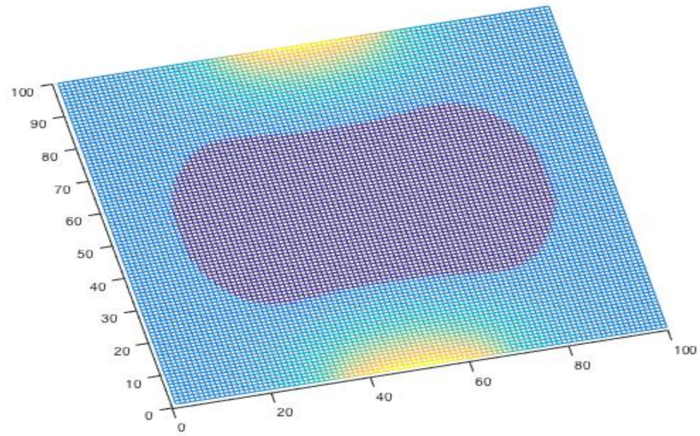

Figure 3.5 Half horizon result

```
%%%% adjoint
R=[]; p=0*E; for kkk=50:-1:1;  E=EE(:,kkk);
%% we must have E (initial condition for the horizon)
for k=1:20; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS; q(j)=rho*cS; q=spdiags(q(:),0,n^2,n^2);
%%%%% Store the solid index jj=[jj j]; (be careful since j has different length)
E=E-q*((q+(kS*dt/2)*h)\(kS*dt*h*T0-dt*u(kkk)*g0(:)));  EEP(:,k)=E;  end
Btp=0;  for k=20:-1:1; p=(q+(kS*dt)*h)\(q*(p+1.e-2*dt*Q*(EEP(:,k)-Eb)));
Btp=Btp+dt*sum(p.*g0(:)); end; R=[Btp R]; end
R=u+R/n^2; g=-R'; eold=g'*g; d=g; v=0*g;

while eold>ep, E=E0; Ep=0*E; for kkk=1:50; EE(:,kkk)=E;  EP(:,kkk)=Ep;
%%%% we must specify control u=g_{kkk}
for k=1:20; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS; q(j)=rho*cS; q=spdiags(q(:),0,n^2,n^2);
%%%%% Store the solid index jj=[jj j]; (be careful since j has different length)
E=E-q*((q+(kS*dt)*h)\(kS*dt*h*T0-dt*u(kkk)*g0(:)));
```

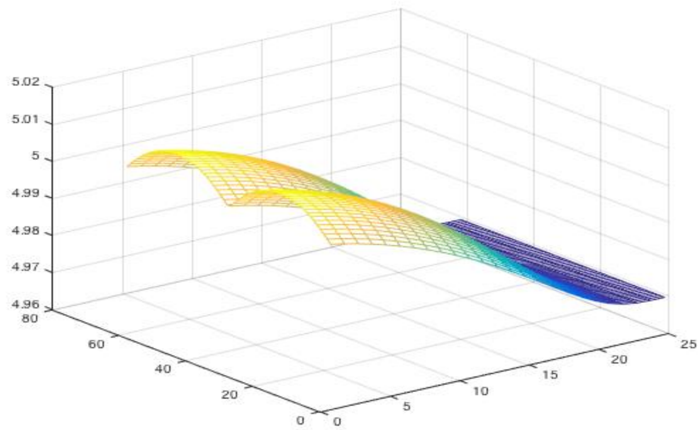

Figure 3.6 The resultant optimal control on the half horizon

```
Ep=q*((q+(kS*dt)*h)\(Ep+dt*d(kkk)*g0(:))); end; end

%%%% adjoint
R=[]; p=0*E; for kkk=50:-1:1;  E=EE(:,kkk); Ep=EP(:,kkk);
%% we must have EE, EEP
for k=1:20; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS; q(j)=rho*cS; q=spdiags(q(:),0,n^2,n^2);
%%%%% Store the solid index jj=[jj j]; (be careful since j has different length)
E=E-q*((q+(kS*dt)*h)\(kS*dt*h*T0-dt*u(kkk)*g0(:)));
Ep=q*((q+(kS*dt)*h)\(Ep+dt*d(kkk)*g0(:)));  EEP(:,k)=Ep; end;
Btp=0; for k=20:-1:1; p=(q+(kS*dt)*h)\(q*(p+1e-2*dt*Q*EEP(:,k)));
Btp=Btp+dt*sum(p.*g0(:)); end; R=[Btp R]; end
%%%%% we claim Lv=R;
%%%%% we claim Ld=R; A=al*I+L (as Av=-R)
Ld=1*d+R'/n^2; al=eold/(d'*Ld); v=v+al*d;  g=g-al*Ld; z=g;  enew=g'*g;
bt=enew/eold; d=g+bt*d; eold=enew;   %k=k+1; E=[E eold];
end
```

Next, we present the half horizon MATLAB code.

```
T=33*ones(n,n); T(k)=25; T=(speye(n^2)+1.e-3*h)\T(:);
```

```
i=find(T(:)>=Tm); E(i)=rho*cL*(T(i)-Tm)+rhoL;
j=find(T(:)<Tm); E(j)=rho*cS*(T(j)-Tm); E=E(:);
g0=zeros(100); g0(1,35:65)=5; g0(end,35:65)=5; g0=n*g0; E0=E;
Q=speye(n^2); u=5*ones(62,25); QQ=zeros(n^2,20);

kmax=25; u=5*ones(62,25); psi=0*E; k=find(abs(Eb)<1000); psi(k)=1;
vv=[]; e0=1e8; for jjj=1:30; E=E0; %we must specify control u=g_{kkk} to compute E
ii=0; for kkk=1:kmax; %%%% we must specify control u=g_{kkk}
g0(1,35:65)=u(1:31,kkk)'; g0(end,35:65)=u(32:62,kkk)';
for k=1:20; ii=ii+1; T0=Tm*ones(n^2,1)+0.e-5*(E-rhoL/2); q=1e5*ones(n^2,1);
i=find(E(:)>=rhoL); T0(i)=Tm+(E(i)-rhoL)/rho/cL; q(i)=rho*cL;
j=find(E(:)<=0); T0(j)=Tm+E(j)/rho/cS;
q(j)=rho*cS; QQ(:,ii)=q; q=spdiags(q,0,n^2,n^2);
%%%%% Store the solid index jj=[jj j]; (be careful since j has different length)
E=E-q*((q+(kS*dt)*h)\(kS*dt*h*T0-dt*n*g0(:))); end; end; Eb=E;
%%%% adjoint
R=[]; p=psi.*(E-Eb); ii=20*kmax+1; for kkk=kmax:-1:1;
%% we must have E (initial condition for the horizon)
Btp=zeros(62,1); for k=20:-1:1; ii=ii-1; q=spdiags(QQ(:,ii),0,n^2,n^2);
p=(q+(kS*dt)*h)\(q*p); pp=reshape(p,n,n);
Btp=Btp+dt*n*[pp(1,35:65) pp(end,35:65)]'; end; R=[Btp R]; end
R=.000001*u+R/n^2; g=-R(:); eold=g'*g, d=g; if eold >e0; break, end;
v=0*g;e0=eold; gg=g; %(Eb=E===> p=0==>R=0)

%while eold>1.e-0,
for iii=1:3; ii=0; Ep=0*E0; dd=reshape(d,62,25); for kkk=1:kmax;
g0(1,35:65)=dd(1:31,kkk)'; g0(end,35:65)=dd(32:62,kkk)';
for k=1:20; ii=ii+1;q=spdiags(QQ(:,ii),0,n^2,n^2);
Ep=q*((q+(kS*dt)*h)\(Ep+dt*n*g0(:))); end; end %%%(what we need is to have q)
%%%% adjoint
R=[]; p=psi.*Ep; ii=20*kmax+1; for kkk=kmax:-1:1; %% we must have EE, EEP
Btp=zeros(62,1); for k=20:-1:1; ii=ii-1; q=spdiags(QQ(:,ii),0,n^2,n^2);
p=(q+(kS*dt)*h)\(q*p); pp=reshape(p,n,n);
Btp=Btp+dt*n*[pp(1,35:65) pp(end,35:65)]';; end; R=[Btp R]; end
%%%%% we claim Ld=R; A=al*I+L (as Av=-R)
```

```
Ld=.000001*d+R(:)/n^2; al=eold/(d'*Ld); v=v+al*d; g=g-al*Ld; z=g; enew=g'*g,
bt=enew/eold; d=g+bt*d; eold=enew; %k=k+1; E=[E eold];
end; beta=0.5; vv=[vv v]; u0=u; u=u+beta*reshape(v,62,25); end
```

Chapter 4

Cahn-Hilliard Navier-Stokes System

In this chapter we focus on the phase-field model of separation of two fluids. Our objective is to control the Cahn-Hilliard Navier-Stokes system by the boundary control of the velocity field, i.e. $v|_{\partial\Omega} = u$, where Ω is a bounded domain with a sufficiently smooth boundary $\partial\Omega$. Phase separation is considerably involved with a lot of important applications in industry. The main equation that describes the phase separation of a binary fluid mixture is the Cahn-Hilliard equations.

The transport Cahn-Hilliard model can be derived as a gradient flow from an energy as

$$\frac{\partial c}{\partial t} + \nabla \cdot J = 0, \tag{4.1}$$

where c is the concentration of the fluid and J is the diffusional mass flux proportional to the gradient of the generalized chemical potential and the transport as

$$J = c\,v - \alpha \nabla w, \tag{4.2}$$

where $\alpha > 0$ is a diffusion coefficient, w is the chemical potential, and v is the transport velocity field. For the material separation of the two-phase system by the Cahn-Hilliard theory, we define the free-energy potential of the concentration c by

$$E(c) = \int_\Omega (\frac{\varepsilon}{2}|\nabla c(x)|^2 + \frac{1}{\varepsilon}F(c))\,dx, \tag{4.3}$$

where $F(c)$ is the free-energy density of the materials, and $\frac{\varepsilon}{2}|\nabla c|^2$ is the kinetic energy when the material is in a transition between two states. The parameter ε is proportional to the thickness of the interface region. The graph of the transition layer is given in Figure (4.1) below. The

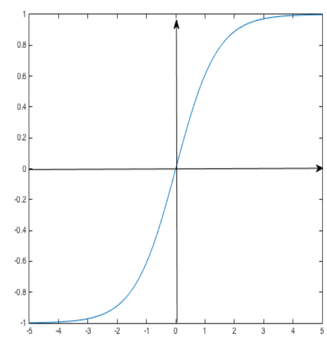

Figure 4.1 The graph of the transition layer

Ginzburg-Landau potential energy corresponds to

$$F(c) = \frac{1}{2}(c^2 - 1)^2. \tag{4.4}$$

Due to the bi-stable potential $F(c)$, solutions of the equation represent a separation of the two fluids. The term $\frac{\varepsilon}{2}|\nabla c(x)|^2$ is added to the energy integral to allow smooth transitions between the two stable states of liquids. This term in the energy forms a diffuse (transition) interface between the two separated states with a profile function, i.e.,

$$c(x) = \tanh(\frac{x}{\sqrt{2\gamma}}), \tag{4.5}$$

satisfying the stationary differential equation

$$\gamma\, c''(x) - (c^2 - 1)c = 0, \tag{4.6}$$

and hence the width of the interfacial layer is $\sqrt{\gamma} = \varepsilon$.
The phase separation process conserves the total mass of concentration c, i.e.

$$\int_\Omega c\, dx = 1, \tag{4.7}$$

so that

$$\frac{d}{dt}\int_{\Omega} c\, dx = 0, \tag{4.8}$$

The chemical potential w is defined by the variational derivative of the energy $E(c)$. That is,

$$(w,h) = \delta E(c)\; h = \lim_{t\to 0}\frac{E(c+t\;h)-E(c)}{t}. \tag{4.9}$$

Thus, the chemical potential w can be written as

$$w = \frac{1}{\varepsilon}F'(c) - \varepsilon\Delta c. \tag{4.10}$$

In order to have conservation of mass, the diffusional mass flux J satisfies the boundary condition

$$n\cdot J = 0, \quad \text{along with} \quad n\cdot\nabla c = 0, \tag{4.11}$$

which prevents the flow of material into or out of the confined volume. For the case $n\cdot v = 0$, i.e. no normal velocity at $\partial\Omega$, and since

$$\frac{\partial}{\partial\nu}F'(c) = F''(c)\frac{\partial c}{\partial\nu}, \tag{4.12}$$

then, the boundary conditions become

$$\frac{\partial c}{\partial\nu} = \frac{\partial}{\partial\nu}w = 0, \quad \text{on } \partial\Omega, \tag{4.13}$$

where $\dfrac{\partial}{\partial\nu}$ is the outward normal derivative at the boundary $\partial\Omega$. Note that, if div $v = 0$, then we have

$$\text{div } J = \text{div }(c\,v - \alpha\nabla w) = -\alpha\Delta w + v\cdot\nabla c.$$

So, we can write the strong form of the transport Cahn-Hilliard equation (4.1) as

$$\frac{\partial c}{\partial t} + v\cdot\nabla c - \alpha\Delta w = 0, \qquad \nabla\cdot v = 0. \tag{4.14}$$

As a consequence, this bi-harmonic flow is the nature of the model of the Cahn-Hilliard system. We have the bi-harmonic diffusion operator $\alpha\Delta^2$, with domain $\dfrac{\partial c}{\partial\nu} = \dfrac{\partial}{\partial\nu}\Delta c = 0$, if $n\cdot v = 0$.

In summary, the strong form of the normalized transport Cahn-Hilliard system is given by

$$\begin{cases} \dfrac{\partial c}{\partial t} + v \cdot \nabla c - \alpha \Delta w = 0, \quad \text{in } \Omega \\ \\ w = -\varepsilon \Delta c + \dfrac{1}{\varepsilon} F'(c), \quad \text{in } \Omega \\ \\ n \cdot \nabla c = 0, \quad n \cdot J = 0, \quad \text{on } \partial\Omega \end{cases} \tag{4.15}$$

Throughout this thesis, and for the sake of simplicity of our presentation, we set the thickness parameter $\varepsilon = 1$ and the conductivity parameter $\alpha = 1$.

4.1 Weak Formulation of Cahn-Hilliard System

In this section we introduce the weak form of the Cahn-Hilliard equations, and then develop the existence theory for dynamics control in Section (4.4). The weak form of the concentration equation (4.1) in c is given by

$$(\frac{d}{dt} c, \psi) + (\text{div } J, \psi) = 0, \quad \forall \, \psi \in H^1(\Omega),$$

which implies, using Green's formula, that

$$(\frac{\partial c}{\partial t}, \psi) - (c\, v - \nabla w, \nabla \psi) = 0, \quad \forall \, \psi \in H^1(\Omega), \tag{4.16}$$

where we used

$$(\text{div } J, \psi) = \int_\Gamma (n \cdot J) \psi \, ds - \int_\Omega J \, \nabla \psi \, dx.$$

and the boundary condition $n \cdot J = 0$. Moreover

$$(J, \nabla \psi) = (c\, v, \nabla \psi) + (w, \Delta \psi).$$

The weak form of the chemical potential equation (4.10) in w is given by

$$(w, \psi) = (-\Delta c, \psi) + (F'(c), \psi),$$

which is derived using Green's formulas as

$$(w, \psi) = (\nabla c, \nabla \psi) + (F'(c), \psi), \quad \forall \, \psi \in H^1(\Omega) \tag{4.17}$$

since $n \cdot \nabla c = 0$.

4.2 Incompressible Flow by Navier-Stokes Equations

In this section we introduce the basic theory of the incompressible flow governed by Navier-Stokes Equations. The equations can be derived from the laws of conservation of mass and conservation of momentum, given by

$$\begin{cases} \dfrac{\partial \rho}{\partial t} + \mathrm{div}(\rho v) = 0, \\ \\ (\rho v)_t + \mathrm{div}(\dfrac{1}{2}\rho |v|^2 - S) = f, \end{cases} \tag{4.18}$$

where $\rho = \rho(t, x)$ is the mass density, $v = v(t, x)$ is the velocity of the fluid over domain $\Omega \in R^d$, and S is the stress tensor defined as

$$S = 2\mu\varepsilon - p\, I, \tag{4.19}$$

where μ is the viscosity, I is the identity matrix, and ε is the linear strain defined by

$$\varepsilon = \frac{1}{2}(\nabla v + \nabla v^t), \tag{4.20}$$

where

$$\varepsilon_{ij} = \frac{1}{2}(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}). \tag{4.21}$$

The Navier-Stokes equation can be written as

$$\rho \frac{Dv}{Dt} + \mathrm{div} S = f, \tag{4.22}$$

where

$$\mathrm{div} S = \Delta v - \nabla p, \tag{4.23}$$

and $\dfrac{Dv}{Dt}$ is the Lagrangian derivative (or total derivative or material derivative) of the velocity, given by

$$\frac{Dv}{Dt} = (\frac{\partial v}{\partial t} + v \cdot \nabla v). \tag{4.24}$$

It is the rate change of the velocity along the flow. It comes from taking the time derivative of $v = v(t, x(t))$ (a function of two variables, time t and position $x(t)$, with $v(t, x(t)) = \frac{dx}{dt}$),

$$\frac{d}{dt}v(t, x(t)) = \frac{\partial v}{\partial t} + v \cdot \nabla v = \frac{Dv}{Dt} \tag{4.25}$$

The transport term $v \cdot \nabla v$ is taken coordinate-wise, i.e.,

$$(v \cdot \nabla v)_j = v \cdot \nabla v_j. \tag{4.26}$$

For example, a two dimensional flow $v = (v^1, v^2)$ in spatial coordinates x_1, x_2 has

$$v \cdot \nabla v = \begin{pmatrix} v^1 \dfrac{\partial v^1}{\partial x_1} + v^2 \dfrac{\partial v^1}{\partial x_2} \\ \\ v^1 \dfrac{\partial v^2}{\partial x_1} + v^2 \dfrac{\partial v^2}{\partial x_2} \end{pmatrix} = \begin{pmatrix} v \cdot \nabla v^1 \\ \\ v \cdot \nabla v^2 \end{pmatrix}$$

Substitute equations (4.23)–(4.24) in equation (4.22), we get

$$\rho(\frac{\partial v}{\partial t} + v \cdot \nabla v) + \nabla p = \mu \Delta v + f, \tag{4.27}$$

where p is the pressure, μ is the viscosity of the medium, and f is the applied force vector.

Incompressible flow means that the mass density of the fluid remains constant during flow motion, so the state equation can be written as

$$\rho = \rho(t, x) = \rho_0, \tag{4.28}$$

for some constant ρ_0. In this case the mass conservation equation (4.18) becomes

$$\text{div } v = \nabla \cdot v = 0. \tag{4.29}$$

So, the incompressible Navier-Stokes equations are given by

$$\rho(\frac{\partial v}{\partial t} + v \cdot \nabla v) + \nabla p = \mu \Delta v + f, \quad \nabla \cdot v = 0, \tag{4.30}$$

where the gradient term ∇p balances the momentum equation for the divergence-free condition. For the coupled Cahn-Hilliard Navier-Stokes system, the fluid structure interaction enters into the Navier-Stokes equations as a force of the form

$$f = -\nabla \cdot (\nabla c \times \nabla c) = -\Delta c \, \nabla c, \tag{4.31}$$

but

$$-\Delta c \, \nabla c = (w - F'(c)) \, \nabla c = w \nabla c - \nabla F(c)$$

and the term $\nabla F(c)$ is absorbed into the pressure term. If we assume normalized mass density ρ, then the strong form of the coupled incompressible Navier-Stokes equations can be written as

$$\frac{\partial v}{\partial t} + v \cdot \nabla v - \mu \Delta v + \nabla p = w \nabla c, \quad \nabla \cdot v = 0, \tag{4.32}$$

The Stokes equation is the massless version (i.e. $\rho = 0$) of the Navier-Stokes equation (4.30), i.e.,

$$\nabla p = \mu \Delta v + f, \quad \nabla \cdot v = 0, \tag{4.33}$$

4.2.1 Navier Boundary Conditions and Slip Functions

The Navier boundary condition states that the velocity on the boundary is proportional to the tangential component of the normal stress, i.e.

$$(S \cdot n)_\tau + \beta \, (\tau \cdot v - g) = 0 \tag{4.34}$$

where $(S \cdot n)_\tau$ is the tangential component of the normal stress, and g is a given function. The normal stress $(S \cdot n) \in L^2(0, T; H^{-1/2}(\Gamma))$. Note that if $\beta \to \infty$ in (4.34), then we get

$$\tau \cdot v = g,$$

and if $\beta = 0$, then we have

$$(S \cdot n)_\tau = 0.$$

In the optimal control analysis, we are interested in the slip boundary conditions, i.e.

$$\begin{cases} \tau \cdot v = g_1, \\ \\ n \cdot v = g_2, \end{cases} \tag{4.35}$$

4.2.2 Weak Formulation of Navier-Stokes Equations

In this section we introduce the weak form for the velocity v of the momentum equation (4.32). The weak form of the velocity is based on the definition of the tri-linear form $b(v, w, \phi)$. We start by introducing the standard divergence-free spaces

$$V_0 = \{v \in H_0^1(\Omega)^d : \nabla \cdot v = 0\},$$

and

$$V = \{v \in H^1(\Omega)^d : \nabla \cdot v = 0\}.$$

Let H_0 and H be the completion of V_0 and V with respect to $L^2(\Omega)^d$, respectively, i.e.

$$H_0 = \{v \in L^2(\Omega)^d : \nabla \cdot v = 0,\ n \cdot v = 0, \text{ on } \partial\Omega\},$$

and

$$H = \{v \in L^2(\Omega)^d : \nabla \cdot v = 0\}.$$

First, we define the tri-linear form $b : V \times V \times V_0 \to \mathbb{R}$ for the convictive term by

$$b(v, w, \phi) = \langle v \cdot \nabla w, \phi \rangle = \int_\Omega (v \cdot \nabla w) \cdot \phi \, dx.$$

It can be shown that the trilinear form b satisfies the following properties
(a) $b(v, w, \phi) + b(v, \phi, w) = 0$, provided that

$$\text{div } v = 0, \text{ and } (n \cdot v)(w \cdot \phi) = 0, \text{ on } \Gamma.$$

(b) $|b(v, w, \phi)| \leq |v|_{L^4} \ |\nabla w|_{L^2} \ |\phi|_{L^4} \leq M \ |v|_V \ |\nabla w|_V \ |\phi|_{V_0}$.

(c) $|b(v, w, \phi)| \leq M_1 \ |v|_{L^2}^{1/2} \ |v|_V^{1/2} \ |\phi|_{L^2}^{1/2} \ |\phi|_{V_0}^{1/2} \ |w|_V$ in 2-D.

(d) $|b(v, w, \phi)| \leq M_1 \ |v|_{L^2}^{1/4} \ |v|_V^{3/4} \ |\phi|_{L^2}^{1/4} \ |\phi|_{V_0}^{3/4} \ |w|_V$ in 3-D.

The weak form of the Navier-Stokes equations can be derived from (4.22), as

$$(\rho \frac{Dv}{Dt}, \phi) + (\text{div} S, \phi) - (f, \phi) = 0, \quad \forall \phi \in V_0, \tag{4.36}$$

which can be written using (4.24), as

$$(\frac{\partial v}{\partial t}, \phi) + (v \cdot \nabla v, \phi) - (\mathrm{div} S, \phi) = (w \nabla c, \phi), \quad \forall \phi \in V_0, \tag{4.37}$$

where

$$(\mathrm{div} S, \phi) = \int_{\partial\Omega} (n \cdot S)\, \phi \, ds - \int_{\Omega} S : \nabla \phi \, dx$$

where we used the Frobenius product defined as

$$\int_{\Omega} S : \nabla \phi \, dx = \sum_{i,j} (S_{ij})(\nabla \phi_{ij}) = (S, \nabla \phi),$$

Using the definition of the Stress tensor, we can write

$$(S, \nabla \phi) = (2\mu\varepsilon - p\, I, \nabla \phi) = 2\mu(\varepsilon, \nabla \phi) + (p\, I, \nabla \phi) = 2\mu(\frac{1}{2}(\nabla v + (\nabla v)^t), \nabla \phi) + (p, \nabla \phi).$$

The term $(p, \nabla \phi)$ vanishes, since $\phi \in V_0$ and

$$(\nabla p, \phi) = \int_{\Omega} \nabla p \, \phi \, dx = \int_{\Gamma} (n \cdot \phi)\, p \, ds - \int_{\Omega} p \, \mathrm{div} \phi \, dx = 0$$

since, $n \cdot \phi = 0$ and $\mathrm{div}\phi = 0$.
Thus,

$$(S, \nabla \phi) = \mu(\nabla v + (\nabla v)^t, \nabla \phi),$$

where

$$\nabla v = \begin{pmatrix} \dfrac{\partial v_1}{\partial x_1} & \dfrac{\partial v_1}{\partial x_2} \\ \\ \dfrac{\partial v_2}{\partial x_1} & \dfrac{\partial v_2}{\partial x_2} \end{pmatrix}$$

and

$$2\mu\, \varepsilon = \begin{pmatrix} \mu \dfrac{\partial v_1}{\partial x_1} + \mu \dfrac{\partial v_1}{\partial x_1} & \mu \dfrac{\partial v_1}{\partial x_2} + \mu \dfrac{\partial v_2}{\partial x_1} \\ \\ \mu \dfrac{\partial v_2}{\partial x_1} + \mu \dfrac{\partial v_1}{\partial x_2} & \mu \dfrac{\partial v_2}{\partial x_2} + \mu \dfrac{\partial v_2}{\partial x_2} \end{pmatrix}$$

and

$$\nabla\phi = \begin{pmatrix} \dfrac{\partial\phi_1}{\partial x_1} & \dfrac{\partial\phi_1}{\partial x_2} \\ \\ \dfrac{\partial\phi_2}{\partial x_1} & \dfrac{\partial\phi_2}{\partial x_2} \end{pmatrix}$$

So, since div $v = 0$, we have

$$(S, \nabla\phi) = \mu(\nabla v, \nabla\phi).$$

Thus, the weak form of the coupled Navier-Stokes equation can be written as

$$(\frac{d}{dt}v, \phi) + b(v, v, \phi) + \mu(\nabla v, \nabla\phi) = (w\nabla c, \phi), \quad \forall\phi \in V_0. \tag{4.38}$$

In summary, the weak form of the coupled system of Cahn-Hilliard Navier-Stokes system can be written as

$$\begin{cases} (\dfrac{d}{dt}v, \phi) + b(v, v, \phi) + \mu(\nabla v, \nabla\phi) = (w\nabla c, \phi), \quad \forall\phi \in V_0 \\ \\ (\dfrac{d}{dt}c, \psi_1) - (c\,v - \nabla w, \nabla\psi_1) = 0, \quad \forall\ \psi_1 \in H^1(\Omega) \\ \\ (\nabla c, \nabla\psi_2) + (F'(c), \psi_2) = (w, \psi_2), \qquad \forall\psi_2 \in H^1(\Omega). \end{cases} \tag{4.39}$$

4.3 Sharpened and Obstacle Ginzburg-Landau Potential

Compared to the weak form given by (4.39), the strong form of the normalized equation of Cahn-Hilliard Navier-Stokes system on Ω can be written as

$$\begin{cases} \dfrac{d}{dt}v + v\cdot\nabla v - \nabla\cdot(\mu(c)\nabla v) + \nabla p = w\nabla c, \quad \nabla\cdot v = 0. \quad \text{in } \Omega, \quad v|_{\partial\Omega} = u, \\ \\ \dfrac{d}{dt}c + v\cdot\nabla c - \alpha\Delta w = 0, \qquad \text{in } \Omega \\ \\ w = -\Delta c + F'_\beta(c), \qquad \text{in } \Omega \\ \\ n\cdot\nabla c = 0, \quad n\cdot J = 0, \qquad \text{on } \partial\Omega \end{cases} \tag{4.40}$$

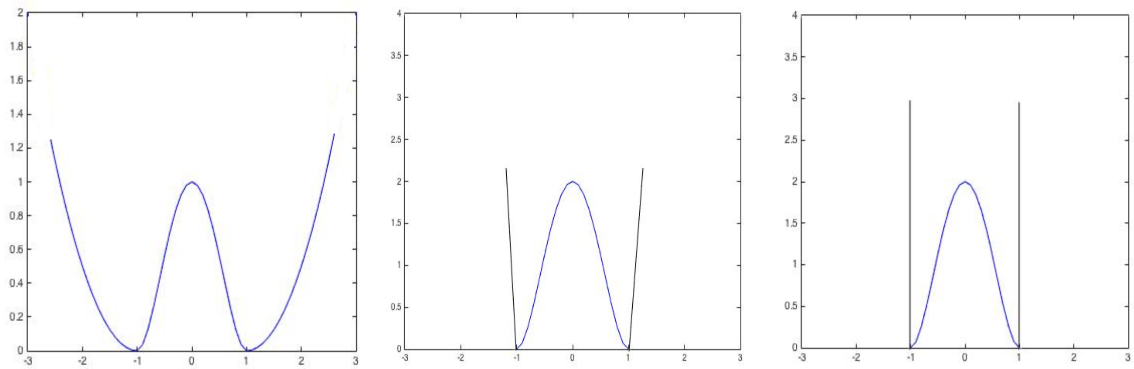

Figure 4.2 Ginzburg-Landau potential: standard-sharp-obstacle

where as we recall, from sections (4.1) and (4.2), that v is the velocity field, $\alpha > 0$ is a diffusion coefficient, p is the pressure, c denotes the concentration, w is the associated chemical potential, $\mu(c)$ is fluid viscosity and $(w\nabla c)$ is the interaction force. The first equation of the system is for fluid velocity v governed by incompressible Navier Stokes equations and the interaction force $(w\nabla c)$. The second equation is for fluid concentration c. It consists of the transport equation of fluid velocity and diffusion by chemical potential w.
The viscosity of fluid $\mu(c)$ can be assumed to be a function of c, for example

$$\mu(c) = \frac{\mu_1(1-c) + \mu_2(c+1)}{2},$$

where $\mu_1,\ \mu_2 > 0$ are the viscosity of the two phases. But, for sake of simplicity we assume that viscosity is constant.
Now, we introduce the sharpened Ginzburg-Landau potential in the free energy $E(c)$, defined in (4.3). For $\beta > 0$, the standard Ginzburg-Landau potential is defined by

$$F_\beta(c) = \begin{cases} \frac{\beta}{2}|c+1|^2 & c \le -1 \\ \\ \dfrac{1}{2}(1-c^2)^2 & c \in [-1,1] \\ \\ \frac{\beta}{2}|c-1|^2 & c \ge 1. \end{cases} \tag{4.41}$$

where $c = \pm 1$ indicate the two fluids domains separate from the transition layer. The derivative of the Ginzburg-Landau potential is

$$F'_\beta(c) = \begin{cases} \beta(c+1) & c \leq -1 \\ \\ -2c\,(1-c^2) & c \in [-1,1] \\ \\ \beta(c-1) & c \geq 1. \end{cases} \tag{4.42}$$

We are interested in the obstacle Ginzburg-Landau potential [36, 37], i.e. $\beta \to \infty$, as shown in Figure (4.2),

$$F'_\beta(c) = \begin{cases} \infty & c < -1 \\ \\ -2c\,(1-c^2) & c \in [-1,1] \\ \\ \infty & c > 1. \end{cases} \tag{4.43}$$

If we let $\beta \to \infty$ we obtain the double obstacle potential law, i.e. $\mathcal{K} = \{c \in H^1(\Omega) : |c| \leq 1\}$ and $c \in \mathcal{K}$ satisfies the variational inequality

$$\langle -\Delta c + F'(c), \tilde{c} - c \rangle \geq 0 \text{ for all } \tilde{c} \in \mathcal{K}.$$

In section (4.7), we will show the existence of a strong form solution of obstacle potential (4.43) with the help of Lagrange multipliers λ in $L^2((0,T) \times \Omega)$ such that

$$\begin{cases} -\Delta c + F'(c) + \lambda = w, \\ \\ \lambda = \max(0, \lambda + c - 1) + \min(0, \lambda + (c+1)). \end{cases}$$

Also, in chapter 5 we will consider the optimal control problem for the boundary velocity control and derive the strong necessary optimality in the form of the Lagrange multiplier.
Our main objective in the analysis of the Cahn-Hilliard Navier-Stokes system is to control the evolution of the separation process by a boundary control of the fluid velocity.

4.4 Constructing a Weak Solution of Cahn-Hilliard Navier-Stokes System

In this section we construct a weak solution of the Cahn-Hilliard Navier-Stokes system (4.39). Since the velocity field does not have a homogeneous boundary conditions, we need to define Green's map of the boundary action, in order to be able to establish a weak solution.
Define the Green's map of the boundary action, $G : u \in H^{1/2}(\Gamma) \to Gu = v \in V$, by

$$(\nabla v, \nabla \phi) = \int_\Omega \nabla v : \nabla \phi \, dx = \sum_k \int_\Omega \sum_{i,j} \frac{\partial v_i}{\partial x_k}, \frac{\partial v_j}{\partial x_k}, \quad \text{and } v|_\Gamma = u, \quad \forall \, \phi \in V_0.$$

Here we used the Trace theorem, which asserts that for all $u \in H^{1/2}(\Gamma)$, there exists $\tilde{v} \in H^1(\Omega)$, such that $\tilde{v}|_\Gamma = u$. Note that Gu is the harmonic extension of $v|_\Gamma$ to the whole domain Ω, where we can decompose v into the sum of a homogeneous part and a boundary part. Hence, we will try to find a solution of the form $v = z + \tilde{v}$, satisfying

$$(\nabla z + \nabla \tilde{v}, \nabla \phi) = 0, \forall \, \phi \in V_0,$$

where $z \in V_0$, $\text{div} z = 0$ and $z|_\Gamma = 0$.
Thus, we can seek a solution of the form $v(t) = z(t) + Gu \in V$ and $z(t) \in V_0$, and show the existence of weak solutions satisfying

$$\langle \frac{d}{dt} z(t), \phi \rangle_{V_0^*, V_0} + b(z(t) + Gu, z(t) + Gu, \phi) + \mu(\nabla z(t), \nabla \phi) - (w \nabla c, \phi) = 0, \quad \forall \, \phi \in V_0, \tag{4.44}$$

where $\text{div}(Gu) = 0$, $\text{div} z = 0$, and $Gu|_\Gamma = v$.
To construct a weak solution of the system (4.39) with (4.44), we follow the well-known Galerkin method by representing the solution in terms of linear combinations of basis functions e_k, ϕ_k, as

$$\begin{cases} z(t) = \displaystyle\sum_{k=1}^{n} z_k(t) e_k, & \text{where } e_k \text{ is a basis of } V_0 \\ c(t) = \displaystyle\sum_{k=1}^{n} c_k(t) \phi_k, & \text{where } \phi_k \text{ is a basis of } H^1(\Omega) \\ w(t) = \displaystyle\sum_{k=1}^{n} w_k(t) \phi_k, & \text{where } \phi_k \text{ is a basis of } H^1(\Omega). \end{cases} \tag{4.45}$$

For example, e_k can be chosen to be the eigenfunctions of Stokes operator and ϕ_k the eigenfunctions of Laplacian operator. Substituting the above equations (4.45) into the system (4.39), and testing against the same element, we get the following Galerkin system

$$\begin{cases} (\frac{d}{dt}(\sum_{k=1}^{n} z_k(t)e_k + Gu_k(t)), e_j) + b(\sum_{k=1}^{n} z_k(t)e_k + Gu_k, \sum_{k=1}^{n} z_k(t)e_k + Gu_k, e_j) \\ \quad +\mu(\nabla \sum_{k=1}^{n} z_k(t)e_k + Gu_k, \nabla e_j) = (\sum_{k=1}^{n} w_k(t)\phi_k \nabla \sum_{k=1}^{n} c_k(t)\phi_k, e_j), \\ (\frac{d}{dt}(\sum_{k=1}^{n} c_k(t)\phi_k), \phi_j) - (\sum_{k=1}^{n}(z_k(t)e_k + Gu_k) \ \sum_{k=1}^{n} c_k(t)\phi_k - \nabla \sum_{k=1}^{n} w_k(t)\phi_k, \nabla\phi_j) = 0, \\ (\sum_{k=1}^{n} w_k(t)\phi_k, \phi_j) = (\nabla \sum_{k=1}^{n} c_k(t)\phi_k, \nabla\phi_j) + (F'(c), \phi_j). \end{cases} \tag{4.46}$$

The above Galerkin system is a linear system of ODE's with a locally Lipschitz RHS. So, by the classical ODE theory, there exists a unique local in time solution of this system.

4.4.1 An Apriori Estimate for the Weak Solution

In order to show the existence of global in time solution, and then pass the limit as $n \to \infty$, we need to find a priori estimate for the weak solution of the Galerkin system (4.46), then we apply Aubin's lemma for existence of the limit as a weak solution for (4.39).

To do so, multiply the first equation in (4.39) by $(z^n(t))$, the second equation in (4.39) by $(w^n(t))$ and the third equation in (4.39) by $(\frac{d}{dt}c^n(t))$

$$\begin{cases} (\frac{d}{dt}(z^n + Gu), z^n) + b(z^n + Gu, z^n + Gu, z^n) \\ \quad +\mu(\nabla(z^n + Gu), \nabla z^n) - (w^n \nabla c^n, z^n) = 0, \\ (\frac{d}{dt}c^n, w^n) - (c^n \ (z^n + Gu) - \nabla w^n, \nabla w^n) = 0, \\ -(w^n, \frac{d}{dt}c^n) + (\nabla c^n, \nabla(\frac{d}{dt}c^n)) + (F'(c^n), \frac{d}{dt}c^n) = 0. \end{cases} \tag{4.47}$$

This is valid since $z^n(t)$ is a linear combination of e_j and $w^n(t)$, $\frac{d}{dt}c^n(t)$ are linear combinations of ϕ_k. Next, adding up the three equation in (4.47) together, we get the following expression

$$(\frac{d}{dt}(z^n + Gu), z^n) + b(z^n + Gu, z^n + Gu, z^n) + \mu(\nabla(z^n + Gu), \nabla z^n) - ((Gu)\, c^n, \nabla w^n)$$

$$+(\nabla w^n, \nabla w^n) + (\nabla c^n, \nabla(\frac{d}{dt}c^n)) + (F'(c^n), \frac{d}{dt}c^n) = 0, \tag{4.48}$$

Here, since $z^n \in V_0$, we have

$$(w^n\, \nabla c^n + c^n\, \nabla w^n, z^n) = (\nabla(c^n + w^n), z^n) = 0.$$

Now, equation (4.48) implies that

$$(\frac{d}{dt}(z^n + Gu), z^n) + b(z^n + Gu, z^n + Gu, z^n) + \mu(\nabla(z^n + Gu), \nabla z^n) - ((Gu)\, c^n, \nabla w^n)$$

$$+(\nabla w^n, \nabla w^n) + \frac{d}{dt}[\frac{1}{2}|\nabla c^n|^2 + \int_\Omega F(c^n)\, dx] = 0. \tag{4.49}$$

Note that, using the properties of the tri-linear form in section (4.3)

$$b(z^n + Gu, z^n + Gu, z^n) = b(z^n, z^n, z^n) + b(z^n, Gu, z^n) + b(Gu, z^n, z^n) + b(Gu, Gu, z^n)$$

$$= b(z^n, Gu, z^n) + b(Gu, Gu, z^n).$$

Now, (4.49) can be written as

$$\frac{d}{dt}[\frac{1}{2}(|z^n|^2 + |\nabla c^n|^2) + \int_\Omega F(c^n)\, dx] + \mu(\nabla z^n, \nabla z^n) + (\nabla w^n, \nabla w^n) + J(u) = 0, \tag{4.50}$$

where J contains boundary terms that depend on control u, i.e.

$$J(u) = (\frac{d}{dt}Gu, z^n) + b(z^n, Gu, z^n) + b(Gu, Gu, z^n) + \mu(\nabla Gu, \nabla z^n) - ((Gu)\, c^n, \nabla w^n). \tag{4.51}$$

Next, in order to obtain the full norm in H^1, multiply $c^n(t)$ to the second equation and $w^n(t)$ to the third equation of the strong form (4.40)

$$\begin{cases} (\frac{d}{dt}c^n, c^n) + (v^n\ \nabla c^n, c^n) + (\nabla w^n, \nabla c^n) = 0, \\ \\ (w^n, w^n) - (\nabla c^n, \nabla w^n) - (F'(c^n), w^n) = 0. \\ \end{cases} \tag{4.52}$$

Then, adding up the two equation in (4.52) together, we get the following expression

$$\frac{d}{dt}(\frac{1}{2}|c^n|^2) + (v^n\ \nabla c^n, c^n) + (w^n, w^n) - (F'(c^n), w^n) = 0. \tag{4.53}$$

Now, add the equations (4.50) and (4.53), we get

$$\begin{aligned} &\frac{d}{dt}[\frac{1}{2}(|z^n|^2 + |c^n|^2 + |\nabla c^n|^2) + \int_\Omega F(c^n)\ dx] + \mu(\nabla z^n, \nabla z^n) + (v^n\ \nabla c^n, c^n) + (w^n, w^n) + (\nabla w^n, \nabla w^n) \\ &\quad -(F'(c^n), w^n) + J(u) = 0, \end{aligned} \tag{4.54}$$

Note that the full norm of ψ in $H^1(\Omega)$ is given by

$$|\psi|^2_{H^1(\Omega)} = (\psi, \psi) + (\nabla\psi, \nabla\psi).$$

Next, we establish an apriori bound in 2-D for terms in $J(u)$ in (4.51). First note that

$$(\frac{d}{dt}Gu, z^n) = 0,$$

since Gu is piecewise constant in time, i.e. $\frac{d}{dt}Gu = 0$. Next, using the inequality

$$\big(\sqrt{\frac{\mu}{2}}\ A\big) \cdot \big(\sqrt{\frac{2}{\mu}}\ B\big) \le \frac{\mu}{4}|A|^2 + \frac{1}{\mu}|B|^2,$$

consider

$$b(z^n, Gu, z^n) \le |z^n|_{H_0}\ |Gu|_V\ |z^n|_{V_0} \le \frac{1}{2}\ (|z^n|^2_{V_0} + |z^n|^2_{H_0}\ |Gu|^2_V) \le \frac{\mu}{4}|z^n|^2_{V_0} + \frac{1}{\mu}|z^n|^2_{H_0}\ |Gu|^2_V,$$

Similarly

$$b(Gu, Gu, z^n) \leq |z^n|_{V_0}\ |Gu|_H\ |Gu|_V \leq \frac{1}{2}\ (|z^n|^2_{V_0} + |Gu|^2_H\ |Gu|^2_V) \leq \frac{\mu}{4}|z^n|^2_{V_0} + \frac{1}{\mu}|Gu|^2_H\ |Gu|^2_V.$$

Also

$$(\nabla Gu, \nabla z^n) \leq |Gu|_V\ |z^n|_{V_0} \leq \frac{1}{2}(|Gu|^2_V + |z^n|^2_{V_0}) \leq \frac{\mu}{4}|z^n|^2_{V_0} + \frac{1}{\mu}|Gu|^2_V.$$

In the 2-D case, we can estimate the following term

$$((Gu)\, c^n, \nabla w^n) \leq |\nabla w^n|\ |c^n|^{1/2}_{H^1}\ |c^n|^{1/2}_{L^2}\ |Gu|^{1/4}_H\ |Gu|^{1/2}_V \leq \frac{1}{4}|\nabla w^n|^2 + |c^n|_{H^1}\ |c^n|_{L^2}\ |Gu|^{1/2}_H\ |Gu|_V$$

$$\leq \frac{1}{4}|\nabla w^n|^2 + M\, |c^n|^2_{H^1}\ |Gu|^{1/2}_H\ |Gu|_V,$$

where we used

$$|c^n|_{L^2} \leq M\, |c^n|_{H^1},$$

and the estimate of the 3-D case is similar (with different exponents), since Gu is piecewise constant in time. Thus, we have

$$|J(u)| \leq \frac{3\mu}{4}|z^n|^2_{V_0} + \frac{1}{\mu}|Gu|^2_V\ \left(|z^n|^2_{H_0} + |Gu|^2_H + 1\right) + |u|_{H^{1/2}(\Gamma)}\ |c^n|^2_{H^1(\Omega)},$$

which implies that

$$\frac{d}{dt}[\frac{1}{2}(|z^n|^2 + |c^n|^2 + |\nabla c^n|^2) + \int_\Omega F(c^n)\ dx] + \mu(\nabla z^n, \nabla z^n) + (w^n, w^n) + (\nabla w^n, \nabla w^n) \leq$$

$$\frac{3\mu}{4}|z^n|^2_{V_0} + \frac{1}{\mu}|Gu|^2_V\ \left(|z^n|^2_{H_0} + |Gu|^2_H + 1\right) + |u|_{H^{1/2}(\Gamma)}\ |c^n|^2_{H^1(\Omega)} + \frac{1}{2}(|w^n|^2 + L^2\ |c^n|^2),$$

using that,

$$|(F'(c^n), w^n)| \leq L|c^n|_{L^2}|w^n|_{L^2} \leq \frac{1}{2}(|w^n|^2 + L^2\ |c^n|^2).$$

where L is the Lipschitz constant for F'. Then, there exits $\alpha \in L^1(0,T)$, such that

$$\frac{d}{dt}[\frac{1}{2}(|z^n|^2 + |c^n|^2 + |\nabla c^n|^2) + \int_\Omega F(c^n)\ dx] + \frac{\mu}{4}(\nabla z^n, \nabla z^n) + (v^n\, \nabla c^n, c^n) + \frac{1}{2}((w^n, w^n) + (\nabla w^n, \nabla w^n))$$

$$\leq \alpha(t)(|z^n|_{H_0} + |c^n|_{H^1(\Omega)}) + \frac{1}{\mu}\, |u|^2. \tag{4.55}$$

where

$$\alpha(t) = |c^n|^2 \ \frac{L^2}{2} + \frac{1}{\mu}|Gu|^2_V.$$

By Grönwall's inequality, we obtain the apriori bound

$$\begin{aligned}
&\frac{1}{2}(|z^n(t)|^2_{H_0} + |c^n(t)|^2_{H^1(\Omega)}) + \int_\Omega F(c^n(t))\ dx + \int_0^t (\frac{\mu}{4}|\nabla z^n|^2 + \frac{1}{2}|w^n|^2_{H^1(\Omega)})\ ds \\
&\quad \leq M\ (|z^n(0)|^2_{H_0} + |c^n(0)|^2_{H^1(\Omega)} + \int_\Omega F(c^n(0))\ dx + \int_0^t |u|^2_{H^{1/2}(\Gamma)}\ ds),
\end{aligned} \tag{4.56}$$

where $M = \dfrac{1}{\mu}$. In 3-D case, we have

$$b(z^n, Gu, z^n) \leq M_1\ |z^n|^{1/2}_{H_0}\ |Gu|_V\ |z^n|^{3/2}_{V_0} \leq \frac{M_1}{2}\ (|z^n|_{H_0}\ |Gu|^2_V + |z^n|^3_{V_0}).$$

Similarly

$$b(Gu, Gu, z^n) \leq M_2\ |z^n|_{V_0}\ |Gu|^{3/2}_H\ |Gu|^{1/2}_V \leq \frac{M_2}{2}\ (|z^n|^2_{V_0}|Gu|^3_H + |Gu|_V).$$

Thus, we have

$$\begin{aligned}
|J(u)| \leq \frac{M_1\ \mu}{4}\ |z^n|_{H_0}\ |Gu|^2_V + \frac{M_1}{\mu}|z^n|^3_{V_0} + \frac{M_2\ \mu}{4}\ |z^n|^2_{V_0}|Gu|^3_H + \frac{M_2}{\mu}|Gu|_V + \frac{\mu}{4}|z^n|^2_{V_0} + \frac{1}{\mu}|Gu|^2_V \\
+|u|_{H^{1/2}(\Gamma)}\ |c^n|^2_{H^1(\Omega)},
\end{aligned}$$

which implies that

$$\begin{aligned}
&\frac{d}{dt}[\frac{1}{2}(|z^n|^2 + |c^n|^2 + |\nabla c^n|^2) + \int_\Omega F(c^n)\ dx] + \mu(\nabla z^n, \nabla z^n) + (w^n, w^n) + (\nabla w^n, \nabla w^n) \leq \\
&\frac{M_1\ \mu}{4}\ |z^n|_{H_0}\ |Gu|^2_V + |z^n|^2_{V_0}(\frac{M_1}{\mu}|z^n|_{V_0} + \frac{\mu}{4}) + \frac{M_2\ \mu}{4}\ |z^n|^2_{V_0}|Gu|^3_H + |Gu|_V(\frac{M_2}{\mu} + \frac{1}{\mu}|Gu|_V) \\
&\qquad +|u|_{H^{1/2}(\Gamma)}\ |c^n|^2_{H^1(\Omega)} + \frac{1}{2}(|w^n|^2 + L^2\ |c^n|^2).
\end{aligned}$$

4.4.2 Applying Aubin's Lemma to Pass the Limit as $n \to \infty$

In the previous section we have established an apriori bound for the weak solution of the Galerkin system. In this section we apply Aubin's lemma, stated in section (2.4), to pass the limit as $n \to \infty$. Recall that we have

$$\begin{cases} v^n = z^n + Gu \to v, \\ \\ v^n \xrightarrow{s} v, \quad \text{in } L^2(0,T;H_0). \end{cases} \tag{4.57}$$

In order to be able to apply Aubin's lemma, we need to show that

$$\begin{cases} v \in L^2(0,T;V_0), \\ \\ \dfrac{dv}{dt} \in L^p(0,T;V_0^*), \end{cases} \tag{4.58}$$

with $p = 2$, for the 2-D case, and $p = \dfrac{4}{3}$ for the 3-D case. Consider

$$|b(z^n + Gu, z^n + Gu, \phi) + (\nabla(z^n + Gu), \phi)| \leq M \ \tilde{\alpha}(t) \ |\phi|_{V_0},$$

where $\tilde{\alpha}(t) \in L^2$ for the 2-D case, and $\tilde{\alpha}(t) \in L^{4/3}$ for the 3-D case where

$$|b(v,v,\phi)| \leq |\phi|_V \ |v|_V^{3/2} \ |v|_H^{1/2}.$$

with

$$|v|_H \leq M, \quad \text{and} \ \int_0^T |v|_V^2 < \infty.$$

So, (4.58) holds, and we can conclude that

$$\begin{cases} v^n \xrightarrow{w} v, \quad \text{in } V_0, \\ \\ v^n \xrightarrow{s} v, \quad \text{in } H_0. \end{cases} \tag{4.59}$$

Next, for $w = -\Delta c + F'(c)$, note that $F(c)$ is Lipschitz, and

$$|c^n|_{H^1}^2 \leq M_1, \quad \text{and} \quad |\nabla c^n|_{L^2} \leq M_2.$$

with

$$w^n \in L^2(0,T;H^1(\Omega)).$$

We want to show that

$$\begin{cases} c^n \in L^2(0,T;H^2(\Omega)), \\ \\ \Delta c^n \in L^2(0,T;L^2(\Omega)), \end{cases} \tag{4.60}$$

Recall from equation (4.15) that

$$\frac{dc}{dt} = \Delta w - v \cdot \nabla c,$$

so, the weak form is

$$(\frac{dc}{dt}, \psi) + (v \cdot \nabla c, \psi) + (\nabla w, \nabla \psi) = 0,$$

with

$$\begin{cases} |\psi|_{L^p} \leq M\ |\psi|_{H^1}, \quad \text{in 2-D}, \quad \forall\ \psi \in H^1(\Omega), \\ \\ |\psi|_{L^6} \leq M\ |\psi|_{H^1}, \quad \text{in 3-D}, \quad \forall\ \psi \in H^1(\Omega). \end{cases}$$

We have for the 2-D case

$$|v|_4\ |\nabla c|_4 \leq |v|_V^{1/2}\ |v|_H^{1/2}\ |\nabla c|_{L^2}^{1/2}\ |\nabla c|_{H^1}^{1/2}.$$

So, we get

$$|(\frac{dc}{dt}, \psi)| = |(v \cdot \nabla c, \psi) + (\nabla w, \nabla \psi)| \leq (|\nabla w| + M\ |v|_V^{1/2}\ |\nabla c|_{H^1}^{1/2})\ |\psi|_{H^1},$$

where

$$M = |v|_H^{1/2}\ |\nabla c|_{L^2}^{1/2} < \infty.$$

The three spaces in Aubin's lemma are specified as

$$H^2(\Omega) \subseteq H^1(\Omega) \subseteq H^1(\Omega)^*.$$

So, we have

$$\begin{cases} c^n \in L^2(0,T;H^2(\Omega)), \\ \\ \dfrac{dc^n}{dt} \in L^2(0,T;H^1(\Omega)^*), \end{cases} \tag{4.61}$$

which enable us to use Aubin's lemma and get

$$\begin{cases} c^n \xrightarrow{s} c \in L^2(0,T;H^1(\Omega)), \\ \\ c^n \xrightarrow{w} c \in L^2(0,T;H^2(\Omega)), \end{cases} \tag{4.62}$$

with

$$\nabla c^n \xrightarrow{w} \nabla c, \quad \text{in } L^\infty(0,T;L^2(\Omega)),$$

also

$$\Delta c^n \xrightarrow{w} \Delta c, \quad \text{in } L^2(0,T;L^2(\Omega)).$$

Thus

$$\nabla c^n \xrightarrow{s} \nabla c, \quad \text{in } L^p(0,T;L^2(\Omega)).$$

Next, for the convictive term, recall (4.57), and consider

$$(v^n\, c^n - \nabla w, \nabla\psi),$$

where we have

$$(v^n\, c^n, \nabla\psi) \to (v\, c, \nabla\psi),$$

using (4.57). Next, for the interaction force, consider

$$|w^n\, \nabla c^n, \phi| \leq |\phi|_{V_0}\, |w^n|_{L^2}\, |\nabla c^n|_{L^2},$$

where

$$|\nabla c^n|_{L^2} \leq M, \quad \text{and} \quad |\phi|_{L^p} \leq |\phi|_{V_0}, \;\; p < \infty,$$

so, we can write

$$|w^n\, \nabla c^n, \phi| \leq M\, |\phi|_{V_0}\, |w^n|_{H^1}\, |\nabla c^n|_{L^2}.$$

Now, for the 2-D case, recall (4.59), and consider

$$|b(z^n, z^n, \phi) - b(z, z, \phi)| = |b(z^n, z^n - z, \phi) + b(z^n - z, z, \phi)| \leq |z^n|_4\, |z^n - z|_4\, |\phi|_{V_0} \to 0,$$

since

$$|z^n - z|_4 \leq |z^n - z|_{V_0}^{1/2}\, |z^n - z|_{H_0}^{1/2} \Longrightarrow |z^n - z|_4 \to 0.$$

Similarly, for the convictive term

$$(v^n \cdot \nabla c^n, \psi) \to (v \cdot \nabla c, \psi) \text{ in } L^1(0,T), \quad \forall\, \psi \in H^1(\Omega).$$

since

$$(v^n \cdot \nabla c^n, \psi) - (v \cdot \nabla c, \psi) = ((v^n - v)\nabla c^n, \psi) + (v^n(\nabla c^n - \nabla c), \psi).$$

Also, we have

$$(w^n \nabla c^n, \phi) - (w \nabla c, \phi) = ((w^n - w)\nabla c, \phi) - (w^n(\nabla c^n - \nabla c), \phi) \ \to 0 \text{ in } L^1(0,T), \quad \forall\, \phi \in V_0.$$

So, we conclude that the weak limit $(z^n, c^n, w^n) \to (z, c, w)$, with

$$\begin{cases} z^n \xrightarrow{w} z \in V_0, \\ \\ z^n \xrightarrow{s} z \in H_0, \\ \\ c^n \xrightarrow{s} c \in L^2(0,T; H^1(\Omega)), \\ \\ w^n \xrightarrow{w} w \in L^2(0,T; H^1(\Omega)). \end{cases} \tag{4.63}$$

is a weak solution of the Cahn-Hilliard Navier-Stokes system (4.39).

4.5 Lipschitz Continuity of Solution with Respect to Velocity Boundary Control

In this section we show a result about the smoothness of Galerkin solutions (4.63). We establish the Lipschitz continuity of solutions (v, c, w) of (4.39) corresponding to control $u \in U$. Let (v, c, w) be a solution of (4.39) corresponding to control u and $(\hat{v}, \hat{c}, \hat{w})$ be a solution corresponding to $\hat{u}$. If we define $\delta z = z - \hat{z}$, $\delta c = c - \hat{c}$, and $\delta w = w - \hat{w}$, then we have

$$\begin{cases} \langle \dfrac{d}{dt}(\delta z(t) + G\delta u), \phi\rangle + b(\delta v, v, \phi) + b(v, \delta v, \phi) + \mu(\delta z + G\delta u, \phi) = (\delta w \nabla c + \hat{w}\nabla \delta c, \phi), \\ \\ \langle \dfrac{d}{dt}(\delta\, c(t)), \psi_1\rangle - (c\,\delta v - \hat{v}\,\delta c - \nabla \delta w, \nabla \psi_1) = 0, \\ \\ (\delta w, \psi_2) = (\nabla \delta c, \nabla \psi_2) + (F'(c) - F'(\hat{c}), \psi_2). \end{cases} \tag{4.64}$$

Letting $\phi = \delta z$, $\psi_1 = \delta w$ and $\psi_2 = \dfrac{d}{dt}\delta c$ in (4.64) and summing up, we obtain

$$\begin{aligned} &\frac{1}{2}\,\frac{d}{dt}(|\nabla \delta c|_{L^2}^2 + |\delta z|_{H_0}^2) + |\nabla \delta w|^2 + \mu\,|\nabla \delta z|^2 + b(\delta z + G\delta u, v, \delta z) + b(v, G\delta u, \delta z) \\ &+\mu(\nabla G\delta u, \nabla \delta z) + (\hat{v}\,\delta c, \nabla \delta w) - (\hat{w}\,\nabla \delta c, \delta z) + (F'(c) - F'(\hat{c}), \frac{d}{dt}\delta c) = 0 \end{aligned} \tag{4.65}$$

Here, since $\delta z \in V_0$, we have

$$-(\delta w\,\nabla c, \delta z) - (\delta z\, c, \nabla \delta w) = -(\delta z, \nabla(c\,\delta w)) = 0.$$

Note that

$$|(\hat{w}\,\nabla \delta c, \delta z)| \leq \frac{1}{2}|\hat{w}|_\infty(|\delta z|_{H_0}^2 + |\nabla \delta c|^2),$$

and

$$|(\hat{z}\,\delta c, \nabla \delta w)| \leq \frac{1}{4}|\nabla \delta w|^2 + |\hat{z}|^2\,|\delta c|^2.$$

Next, we estimate terms that depend on δu as follows

$$|(c\,G\delta u, \nabla \delta w)| \leq \frac{1}{4}|\nabla \delta w|^2 + M\,|c|_{H^1}\,|\delta u|^2$$

$$|b(G\delta u, v, \delta z) + b(v, G\delta u, \delta z)| \leq \frac{\mu}{4}|\nabla \delta z|^2 + \frac{1}{\mu}|v|_H\,|v|_V\,|G\delta u|_H\,|G\delta u|_V,$$

and also

$$\mu(\nabla G\delta u, \nabla \delta z) \leq \frac{\mu}{4}|\nabla \delta z|^2\,|\nabla G\delta u|^2.$$

Lastly, using equation (4.1) we have

$$(F'(c) - F'(\hat{c}), \frac{d}{dt}(c - \hat{c})) = (F'(c) - F'(\hat{c}), \operatorname{div}(c\,v - \hat{c}\,\hat{v} - \nabla \delta w). \tag{4.66}$$

Using integration by parts in (4.66), we have

$$
\begin{aligned}
&(\nabla(F'(c)-F'(\hat{c})),(c\,v-\hat{c}\,\hat{v}-\nabla\delta w) \le |F''(c)\,\nabla c-F''(\hat{c})\,\nabla\hat{c}|^2 \\
&\le \frac{1}{4}|\nabla\delta w|^2+\frac{1}{4}|c\,\delta v+\hat{v}\,\delta c|^2,
\end{aligned}
\tag{4.67}
$$

where

$$|c\,\delta v|^2 \le |\delta v|_H^2\ |c|_\infty^2,$$

and

$$|\hat{v}\,\delta c|^2 \le |\hat{v}|_V^2\ |\delta c|_{H^1}^2,$$

So, from equation (4.67), we have

$$|F''(c)\,\nabla c-F''(\hat{c})\,\nabla\hat{c}| \le M\ |v\,\delta c|_{H^2}^2.$$

Hence, it follows from equation (4.65) that

$$
\begin{aligned}
&\frac{1}{2}\frac{d}{dt}(|\nabla\delta c|_{L^2}^2+|\delta z|_{H_0}^2)+\frac{1}{4}(|\nabla\delta w|^2+\mu\,|\nabla\delta z|^2) \\
&\le \alpha(t)(|\nabla\delta c|_{L^2}^2+|\delta z|_{H_0}^2)+M\,|\delta G u|_V^2,
\end{aligned}
\tag{4.68}
$$

for some $M>0$ and $\alpha\in L^1(0,T)$. By Grönwall's inequality, we obtain

$$|\nabla\delta c(t)|_{L^2}^2+|\delta z(t)|_{H_0}^2+\int_0^T\frac{1}{4}(|\nabla\delta w|^2+\mu\,|\nabla\delta z|^2)\,dt \le \tilde{M}\sum_k|\delta u_k|_{H^{1/2}}\Delta t. \tag{4.69}$$

4.6 Semi-Group Analysis for Cahn-Hilliard Equations

In this section we analyze the Cahn-Hilliard equations using the semi-group theory [46]. First, we study the nonlinear semi-group theory. We show that the nonlinear operator for the Cahn-Hilliard equations generates a nonlinear semi-group on $X=L^2(\Omega)$. Second, we use the linear semi-group theory to study the bi-harmonic operator. We prove that the bi-harmonic operator generates an analytic (in time) semi-group on $X=L^2(\Omega)$. Then, based on the semi-group theory we prove a regularity result about $c(t)$ and show how smooth $c(t)$ can be.

4.6.1 Nonlinear Semi-Group Theory for Cahn-Hilliard Equations

Define the nonlinear operator for the Cahn-Hilliard equations (4.15) as

$$A(c) = \Delta(\gamma\Delta c - F'(c)), \tag{4.70}$$

where $F'(c)$ is Lipschitz, and

$$\mathrm{dom}(A) = \{c \in H^4(\Omega) : \frac{\partial}{\partial\nu}c = 0, \frac{\partial}{\partial\nu}\Delta c = 0\}. \tag{4.71}$$

The constant γ is called the interface constant with $\sqrt{\gamma}$ is the width of the interface layer as discussed when we introduced the Cahn-Hilliard equations. Recall from (4.12)–(4.13) that $(\frac{\partial}{\partial\nu}\Delta c = 0)$ is true since $(\frac{\partial}{\partial\nu}w = 0)$, $w = -\Delta c + F'(c)$ and $F'(c)$ is Lipschitz. The Lipschitz condition on F' is

$$|F'(c_1) - F'(c_2)| \leq L|c_1 - c_2|, \tag{4.72}$$

where L is the Lipschitz constant of $F'(c)$. Then

$$\langle A(c_1) - A(c_2), c_1 - c_2\rangle = \langle \Delta(\gamma\Delta c_1 - F'(c_1)) - \Delta(\gamma\Delta c_2 - F'(c_2)), c_1 - c_2\rangle.$$

Applying Green's Identity twice and using $\frac{\partial}{\partial\nu}(c_1 - c_2) = 0$ and $\frac{\partial}{\partial\nu}(F'(c_1) - F'(c_2)) = 0$, we get

$$\langle A(c_1) - A(c_2), c_1 - c_2\rangle = \langle \gamma\Delta(c_1 - c_2), \Delta(c_1 - c_2)\rangle - \langle F'(c_1) - F'(c_2), \Delta(c_1 - c_2)\rangle$$

which simplifies to

$$\langle A(c_1) - A(c_2), c_1 - c_2\rangle = \gamma|\Delta(c_1 - c_2)|^2 - \langle F'(c_1) - F'(c_2), \Delta(c_1 - c_2)\rangle.$$

Then, using (4.72), we conclude

$$\begin{aligned}\langle A(c_1) - A(c_2), c_1 - c_2\rangle &= \gamma|\Delta(c_1 - c_2)|^2 - \langle F'(c_1) - F'(c_2), \Delta(c_1 - c_2)\rangle \\ &\geq \gamma|\Delta(c_1 - c_2)|^2 - L|c_1 - c_2|\,|\Delta(c_1 - c_2)|,\end{aligned} \tag{4.73}$$

where L is the Lipschitz constant of $F'(c)$. Thus, $\exists\omega > 0$ such that

$$\langle A(c_1) - A(c_2), c_1 - c_2\rangle + \omega|(c_1 - c_2)|^2 \geq \frac{\gamma}{2}|\Delta(c_1 - c_2)|^2 \tag{4.74}$$

$\forall\ c_1, c_2 \in dom(A)$ in $X = L^2(\Omega)$. Thus, it follows from [46] that A generates a non-linear semi-group on X.

4.6.2 Linear Semi-Group Theory

In this section we consider the bi-harmonic operator

$$A_0 c = \Delta(\gamma \Delta c), \tag{4.75}$$

with

$$\mathrm{dom}(A_0) = \{c \in H^4(\Omega) : \frac{\partial}{\partial \nu} c = 0, \frac{\partial}{\partial \nu} \Delta c = 0\}, \text{ in } X = L^2(\Omega). \tag{4.76}$$

We show that $-A_0$ generates an analytic (in time) semi-group $S(t)$ on $X = L^2(\Omega)$. In fact, since

$$(A_0 c, c) = \gamma |\Delta c|^2, \quad c \in \mathrm{dom}(A_0), \tag{4.77}$$

then, it follows from [46] that $-A_0$ generates an analytic in time semi-group on $X = L^2(\Omega)$.

4.6.3 Lifting Regularity of c(t)

Now, based on the introduction of the semi-group $S(t)$, one can write solutions to the Cahn-Hilliard equations (4.15) by the variational of constant formula given by

$$c(t) = S(t)c(0) + \int_0^t S(t-s)\ f(s)\ ds, \tag{4.78}$$

where the force $f(s) = f_1(s) + f_2(s)$. The first force $f_1(s)$ is due to the transport and given by $f_1(s) = -v(s) \cdot \nabla c(s)$, whereas the second force $f_2(s)$ is due to Ginzburg-Landau potential force given by $f_2(s) = \gamma \Delta F'(c(s))$. So,

$$f(s) = -v(s) \cdot \nabla c(s) + \gamma \Delta F'(c(s)). \tag{4.79}$$

The linear analytic semi-group $S(t)$ satisfies

$$|A_0^\alpha\ S(t)| \le \frac{M_\alpha}{t^\alpha}, \quad \forall\ \alpha > 0,\ t > 0, \tag{4.80}$$

where A_0^α is the α-fractional power of the positive self-adjoint operator A_0, and

$$\begin{cases} \mathrm{dom}(A_0) = \{c \in H^4(\Omega) : \dfrac{\partial c}{\partial \nu} = 0,\ \dfrac{\partial}{\partial \nu}\Delta c = 0\}, \\ \\ \mathrm{dom}(A_0^{1/2}) = \{c \in H^2(\Omega) : \dfrac{\partial c}{\partial \nu} = 0\}, \\ \\ \mathrm{dom}(A_0^{1/4}) = H^1(\Omega), \\ \\ \mathrm{dom}(A_0^0) = L^2(\Omega). \end{cases} \tag{4.81}$$

So, at a certain fraction α, the domain stops carrying the homogeneous flux property. In general, we have

$$\mathrm{dom}(A_0^\alpha) \subseteq H^{4\alpha}(\Omega). \tag{4.82}$$

Recall that

$$\frac{dc}{dt} = \Delta w - v \cdot \nabla c \ \text{ and } \ w = -\Delta c + F'(c),$$

so, we can write

$$-\frac{dc}{dt} = \Delta\Delta c - \Delta F'(c) + v \cdot \nabla c.$$

Now, since F' is Lipschitz, then

$$|F''(c)| \leq M,$$

thus, we have

$$|(f_2(s), \phi)| = |(-\Delta F'(c), \phi)| = |(\nabla F'(c), \nabla \phi)| = |(F''(c)\nabla c, \nabla \phi)| \leq M\ |\nabla c|\ |\nabla \phi|, \quad \forall\ \phi \in H^1(\Omega).$$

So, we get

$$f_2(s) = -\Delta F'(c) \in \mathrm{dom}(A_0^{-\alpha}), \quad \text{where } \ \alpha = \frac{1}{4}, \tag{4.83}$$

i.e.,

$$|f_2(s)|_{\mathrm{dom}(A_0^{-\alpha})} < \tilde{M}. \tag{4.84}$$

Now, by (4.80), we have

$$|A_0^{\alpha+\beta}\ S(t-s)| \leq \frac{M}{(t-s)^{\alpha+\beta}}. \tag{4.85}$$

So, we get

$$\left| A_0^\beta \int_0^t S(t-s)|\ f_2(s)\ ds \right| = \left| \int_0^t A_0^\beta\ S(t-s)|\ f_2(s)\ ds \right|$$

$$= \int_0^t |A_0^{\alpha+\beta}\ S(t-s)|\ |A_0^{-\alpha}\ f_2(s)|\ ds \leq \int_0^t \frac{M_{\alpha+\beta}}{(t-s)^{\alpha+\beta}}\ |f_2(s)|\ ds \leq M\ \tilde{M}\ \frac{t^{1-(\alpha+\beta)}}{\alpha+\beta-1},$$

where $\alpha+\beta<1$. Thus,

$$\int_0^t S(t-s)\ f(s)\ ds \in \mathrm{dom}(A_0^{\beta}) \subseteq H^{4\beta}(\Omega), \tag{4.86}$$

where

$$\alpha+\beta<1 \Rightarrow \beta<3/4, \quad \text{since } \ \alpha=\frac{1}{4}. \tag{4.87}$$

Next, for the transport force $f_1(s)$, and using $|\nabla c|_{L^2(\Omega)} \leq M$, we have

$$\text{in 2-D: } \ (v\cdot\nabla c,\phi) \leq |v|_H\ |\nabla c|_{L^2(\Omega)}\ |\phi|_{H^{1+\delta}} \leq M\ |\phi|_{H^{1+\delta}}, \tag{4.88}$$

$$\text{in 3-D: } \ (v\cdot\nabla c,\phi) \leq |v|_H\ |\nabla c|_{L^2(\Omega)}\ |\phi|_{H^{\gamma}} \leq M\ |\phi|_{H^{\gamma}}, \tag{4.89}$$

where by (4.87), we have in the 2-D case

$$\alpha=\frac{1+\delta}{4} \Rightarrow \beta<\frac{3-\delta}{4}, \tag{4.90}$$

and in the 3-D case

$$\alpha=\frac{\gamma}{4} \Rightarrow \beta<1-\frac{\gamma}{4}. \tag{4.91}$$

So, by the variational of constant formula (4.78), we get

$$c(t) \in C(0,T;H^{3-\delta}(\Omega)) \cap L^2(0,T;H^5(\Omega)). \tag{4.92}$$

Now,

$$|\nabla c|_{L^2} \leq M \Longrightarrow \int_0^t S(t-s)\ f_2(s)\ ds \subseteq H^{3-\delta}(\Omega), \tag{4.93}$$

$$|\nabla c|_{L^2} \leq M \Longrightarrow \int_0^t S(t-s)\ f_1(s)\ ds \subseteq H^{4\beta}(\Omega). \tag{4.94}$$

Then, using

$$|c|_{H^2} \leq M \Longleftrightarrow |\nabla c|_{H^1} \leq M, \tag{4.95}$$

we get

$$|\Delta F'(c)|_{L^2} = |\nabla F''(c)\ \nabla c| = |\nabla F''(c)\ \nabla c + F''(c)\ \Delta c| \leq M, \tag{4.96}$$

which implies that $\beta < 1$, and

$$\int_0^t S(t-s)\ f_1(s)\ ds \subseteq H^{4\beta}(\Omega). \tag{4.97}$$

For the transport force in 2-D, we have

$$(v \cdot \nabla c, \phi) \leq |v|_H\ |\nabla c|_{H^{1+\delta}}\ |\phi|_{L^2}, \tag{4.98}$$

where

$$|\nabla c|_{H^{1+\delta}} = |c|_{H^{2+\delta}} \subseteq H^{4\beta}(\Omega),$$

so, we get

$$\int_0^t S(t-s)\ f_1(s)\ ds \subseteq H^{4\beta}(\Omega), \quad \beta < 1. \tag{4.99}$$

Now, consider

$$\nabla(v \cdot \nabla c) = \nabla v \cdot \nabla v + v\Delta c \quad \in L^2$$

So, we have

$$(v \cdot \nabla c, \phi) \leq M\ |\phi|_{H^1(\Omega)^*}. \tag{4.100}$$

Thus,

$$\int_0^t |A_0\ S(t-s)\ f(s)|\ ds \leq M_1\ |f_2(s)|^2_{\mathrm{dom}(A_0^{-1/2})},$$

and

$$\int_0^t |A_0^{5/4}\ S(t-s)\ f(s)|\ ds = \int_0^t |A_0\ S(t-s)\ A_0^{1/4}\ f(s)|\ ds \leq M_2\ |f_2(s)|^2_{\mathrm{dom}(A_0^{-1/4})}.$$

So, we conclude that

$$c(t) \in C(0,T; H^3(\Omega)) \cap L^2(0,T; H^5(\Omega)). \tag{4.101}$$

4.7 $L^2(0, T \times \Omega)$ Lagrange Multiplier for Obstacle Potential

In this section we study the limit of the Cahn-Hilliard Navier-Stokes model (4.40) as $\beta \to \infty$ for the sharpened Ginzburg-Landau potential F_β in (4.41). From the third equation in (4.40)

$$|w|^2 = \int_\Omega (|\Delta c|^2 + 2F''_\beta(c)|\nabla c|^2 + |F'_\beta(c)|^2)\, dx, \tag{4.102}$$

where the second derivative of $F_\beta(c)$ is given by

$$F''_\beta(c) = \begin{cases} \beta & |c| > 1 \\ \\ 6c^2 - 2 & |c| < 1. \end{cases}$$

Thus, since $|\nabla c|$ is bounded and $F''_\beta(c)$ is also bounded, and from (4.102) we have

$$\int_0^T \int_\Omega (|\Delta c|^2 + |F'_\beta(c)|^2)\, dx\, dt \quad \text{is bounded uniformly in } \beta > 0. \tag{4.103}$$

Also, since, from the energy estimate, $F_\beta(c)$ is bounded, we have

$$\beta\,(|(c+1)^-|^2 + |(c-1)^+|^2) \quad \text{is uniformly bounded in } L^2(\Omega), \tag{4.104}$$

thus, we have

$$\lambda_\beta = F'_\beta(c) \quad \text{is uniformly bounded in } L^2((0,T)\times\Omega). \tag{4.105}$$

Now, let

$$\tilde{F}_\beta(c) = \begin{cases} \frac{\beta}{2}|c+1|^2 & c \le -1 \\ \\ 0 & c \in [-1,1] \\ \\ \frac{\beta}{2}|c-1|^2 & c \ge 1 \end{cases}$$

Since $(-\Delta + \tilde{F}''_\beta)$ is monotone and $F''_\beta - \tilde{F}''_\beta$ is uniformly bounded, it follows that

$$\int_0^T |c|^2_{H^3}\, dt \le M \int_0^T |\nabla w|^2\, dt$$

for some M independent of β. For $\beta > 0$ let $(v_\beta, c_\beta, w_\beta)$ denote the weak solution to the system (4.39). Then, from equation (4.104), we have

$$|(c_\beta + 1)^-|^2 + |(c_\beta - 1)^+|^2 \to 0, \quad \text{as } \beta \to \infty,$$

and thus, we have

$$\begin{aligned} &c_\beta \to c \in [-1,1] \quad \text{strongly in } L^2(\Omega), \\ &\lambda_\beta \to \lambda \quad \text{weakly in } L^2((0,T)\times\Omega), \end{aligned} \tag{4.106}$$

where λ is called L^2 Lagrange multiplier. Then, using similar argument to showing existence of weak solution and Lipschitz continuity in sections (4.4) and (4.5), we obtain the limiting equations

$$\begin{cases} \dfrac{d}{dt}v + v\cdot\nabla v - \Delta v + \nabla p = w\nabla c, \quad \nabla\cdot v = 0 \\ \\ \dfrac{d}{dt}c - \Delta w + v\cdot\nabla c = 0, \\ \\ -\Delta c + F'(c) + \lambda = w, \quad |c| \le 1, \\ \\ \lambda = \max(0, \lambda + c - 1) + \min(0, \lambda + c + 1). \end{cases} \tag{4.107}$$

The complementarity condition

$$\lambda = \max(0, \lambda + c - 1) + \min(0, \lambda + c + 1), \tag{4.108}$$

follows from the fact that

$$(\lambda_\beta, (c_\beta + 1)^-) + (\lambda_\beta, (c_\beta - 1)^+) \ge 0, \tag{4.109}$$

which converges to 0 in $L^2((0,T)\times\Omega)$ as $\beta\to\infty$, i.e.

$$(\lambda, (c+1)^-) + (\lambda, (c-1)^+) \to 0 \quad \text{in} \quad L^2((0,T)\times\Omega) \quad \text{as} \ \beta\to\infty. \tag{4.110}$$

From the complementarity condition (4.108), we have

$$\begin{cases} \text{if} \quad -1 < c < 1, \quad \text{then} \quad \lambda = 0, \\ \\ \text{if} \ \ c = -1, \quad \text{then} \quad \lambda \le 0, \\ \\ \text{if} \ \ c = 1, \quad \text{then} \quad \lambda \ge 0. \end{cases}$$

Chapter 5

Optimal Control Problem and Necessary Optimality for Cahn-Hilliard Navier-Stokes System

In the previous chapter we have established the existence of weak solutions to the Cahn-Hilliard Navier-Stokes system with boundary control. In this chapter we consider the optimal control formulation of the Cahn-Hilliard Navier-Stokes system (4.40) by the boundary control of the velocity v. We consider the optimal control problem of tracking type of the form

$$\min J(v,c,u) = \frac{1}{2}\int_0^T \left(\int_\Omega (|v-v_d|^2 + |c-c_d|^2)\, dx + \frac{\alpha}{2}\int_\Gamma |u|^2\, ds_x \right) dt, \tag{5.1}$$

over admissible control $u \in U_{ad} = \{u : \sum_{k=0}^{n} |u_k|^2\, \Delta t \le \gamma\}$, subject to the Cahn-Hilliard Navier-Stokes control system (4.39), where v_d, c_d is a desired target state for the velocity field v and concentration c, respectively.

In order to analyze the optimal control problem (5.1), we note that (5.1) can be formulated as the following constraint minimization problem

$$\min F(y) + H(u), \quad \text{subject to } E(y,u) = 0,\ u \in U_{ad} \tag{5.2}$$

where $y = (v,c,w) \in Y$ is the state variable and $u \in U_{ad}$ is the boundary control, and the equality constrain $E(y,u) = 0$ is the control system described by the weak system of Cahn-Hilliard Navier-Stokes equations (4.39).

In this chapter we show the existence of solutions to the optimal control problem (5.1). As we recall from section (3.1) for the thermal control, we step through to first show the weak continuity of the equality constraint in order to establish the existence of optimal control. We also show the existence of solution to the adjoint equation by the standard Galerkin method. Then, we use Lagrange Calculus to derive the necessary optimality. We also develop the sequential programming method to solve the optimal control problem based on the optimality condition. We conclude the chapter by introducing numerical methods to actually compute the optimal boundary control. Our numerical analysis is based on the variational difference method to discretize the free energy functional (4.3) for the Cahn-Hilliard system.

5.1 Existence of optimal controls

Recall that we have established the existence of weak solutions of control problem for (4.40) in section (4.4). In this section we show the weak continuity of equality constraint $E(y, u) = 0$ for $y = (v, c, w) \in Y$, given $u \in U_{ad}$, i.e. the system of weak equations (4.39), in which

$$\begin{cases} v \in H^1(0, T; V_0^*) \cap L^2(0, T; V), \\ \\ c \in L^2(0, T; H^2(\Omega)) \cap H^1(0, T; H^1(\Omega)^*), \\ \\ w \in L^2(0, T; H^1(\Omega)). \end{cases} \tag{5.3}$$

Since the functional $J(y, u)$ in (5.1) is quadratic, then it is coercive and convex in (y, u). Thus, $J(y, u)$ is a weakly lower semi-continuous functional. If we establish the weak continuity of equality constraint $E(y, u)$, i.e. if $y_n \xrightarrow{w} \bar{y}$ and $u_n \xrightarrow{w} \bar{u}$, satisfying $E(y_n, u_n) = 0$, then $(\bar{y}, \bar{u})$ satisfies the constraint

$$E(\bar{y}, \bar{u}) = 0,$$

then we are able to establish the existence of optimal control $u \in U_{ad}$ as discussed in section (3.1).

5.1.1 Weak Continuity of Equality Constraint

In this section we show the weak continuity of equality constraint $E(y,u)$. Let $y^n = (v^n, c^n, w^n) \in Y$ be the corresponding solution to $u_n \in U_{ad}$ of $E(y,u) = 0$, i.e.

$$\begin{cases} (\dfrac{d}{dt}v, \phi) + b(v,v,\phi) + \mu(\nabla v, \nabla \phi) = (w\nabla c, \phi), \quad \forall \phi \in V_0 \\[2ex] (\dfrac{d}{dt}c, \psi_1) - (c\ v - \nabla w, \nabla \psi_1) = 0, \quad \forall\ \psi_1 \in H^1(\Omega) \\[2ex] (\nabla c, \nabla \psi_2) + (F'(c), \psi_2) = (w, \psi_2), \qquad \forall \psi_2 \in H^1(\Omega). \end{cases} \tag{5.4}$$

Since $y^n = (v^n, c^n, w^n)$ in (5.3) is uniformly bounded in n by the apriori bound we have established in section (4.4), then we can establish

$$\begin{cases} b(v^n, v^n, \phi) \to b(\bar{v}, \bar{v}, \phi), \quad \text{in } L^1(0,T)\ \forall\ \phi \in V_0, \\[2ex] (w^n \nabla c^n, \phi) \to (\bar{w}\nabla \bar{c}, \phi), \quad \text{in } L^1(0,T)\ \forall\ \phi \in V_0, \\[2ex] (c^n\ v^n, \psi) \to (\bar{c}\ \bar{v}, \psi), \quad \text{in } L^1(0,T)\ \forall\ \psi \in H^1(\Omega). \end{cases} \tag{5.5}$$

which follows from the previous argument in section (4.4) for the existence of weak solution. Thus, we conclude that $\bar{y} = (\bar{v}, \bar{c}, \bar{w})$, satisfies the constraint $E(\bar{y}, \bar{u}) = 0$.

5.2 Necessary Optimality Using Lagrange Calculus

In this section we apply the Lagrange calculus [47] discussed in Appendix B, to derive the necessary optimal condition for the Cahn-Hilliard Navier-Stokes control system (4.40). For the state and control $(y,u) = (v,c,w,u)$ and the Lagrange multiplier $p = (\pi, \xi, \eta)$, define the Lagrangian functional as

$$\begin{aligned} \mathcal{L}(v,c,w,\pi,\xi,\eta) = J(v,c,u) + \int_0^T \big(\langle \frac{d}{dt}v + v\cdot\nabla v - \operatorname{div} S - w\nabla c, \pi\rangle \\ + \langle \frac{d}{dt}c + \nabla\cdot(c\,v - \nabla w), \xi\rangle + (-\Delta c + F'(c) - w, \eta)\big)\, dt. \end{aligned} \tag{5.6}$$

For all direction $\dot{v} \in W(0,T) = L^2(0,T;V) \cap H^1(0,T;V_0^*)$, we get

$$\mathcal{L}_v(\dot{v}) = \int_0^T (\langle \frac{d}{dt}\dot{v}, \pi\rangle + (\dot{v}\cdot\nabla v + v\cdot\nabla\dot{v}, \pi) + \mu\,(\nabla\dot{v}, \nabla\pi) - (c\,\dot{v}, \nabla\xi) + (v - v_d, \dot{v}))\,dt = 0. \quad (5.7)$$

For all direction $\dot{c} \in W_2(0,T) = L^2(0,T;H^1(\Omega)) \cap H^1(0,T;H^1(\Omega)^*)$, we get

$$\mathcal{L}_c(\dot{c}) = \int_0^T (\langle \frac{d}{dt}\dot{c}, \xi\rangle - (v\dot{c}, \nabla\eta) - (w\nabla\dot{c}, \pi) + (F''(c)\dot{c}, \eta) + (\nabla\eta, \nabla\dot{c}) + (c - c_d, \dot{c}) = 0. \quad (5.8)$$

For all direction $\dot{w} \in L^2(0,T;L^2(\Omega))$, we get

$$\mathcal{L}_w(\dot{w}) = \int_0^T ((\nabla\dot{w}, \nabla\xi) - (\dot{w}\nabla c, \pi) - (\dot{w}, \eta))\,dt = 0. \quad (5.9)$$

Hence, we obtain the adjoint equations for $p = (\pi, \xi, \eta)$ as

$$\begin{cases} -\langle \frac{d}{dt}\pi, \phi\rangle + b(v,\phi,\pi) + b(\phi,v,\pi) + \mu\,(\nabla\pi, \nabla\phi) - (\phi\,c, \nabla\xi) + (v - v_d, \phi) = 0, \qquad \pi(T) = 0, \forall\,\phi \in V, \\[2ex] -\langle \frac{d}{dt}\xi, \psi_1\rangle - (v\cdot\nabla\xi, \psi_1) - (w\,\nabla\psi_1, \pi) + (\nabla\eta, \nabla\psi_1) + (F''(c)\eta, \psi_1) \\[2ex] \qquad +(c - c_d, \psi_1), \qquad \xi(T) = 0, \;\; \forall\,\psi_1 \in H^1(\Omega), \\[2ex] -(\eta, \psi_2) + (\nabla\xi, \nabla\psi_2) - (\pi\cdot\nabla c, \psi_2) = 0, \; \forall\,\psi_2 \in H^1(\Omega). \end{cases} \quad (5.10)$$

In section (5.2), we will show the existence of solution $p = (\pi, \xi, \eta)$ for the adjoint system (5.10) by the Galerkin method as in section (3.2). Let T be the stress for the dual system given as

$$T = \mu\,(\nabla\pi + \nabla\pi^t) - q\,I. \quad (5.11)$$

Then, the strong form of the adjoint equations (5.10) is

$$\begin{cases} -\frac{d}{dt}\pi + v\cdot\nabla\pi - \operatorname{div}(T) - c\,\nabla\xi + v - v_d = 0, \\[2ex] -\frac{d}{dt}\xi - v\cdot\nabla\xi - \Delta\eta + F''(c)\eta + c - c_d = 0, \\[2ex] -\Delta\xi - \pi\cdot\nabla c - \eta = 0. \end{cases} \quad (5.12)$$

Moreover, since

$$\mathcal{L}_u((v,c,w),u,(\pi,\xi,\eta))(u-u^*) = \int_\Gamma \big(\alpha\, u_k^* - \frac{1}{\Delta t}\int_{t_{k-1}}^{t_k} T\cdot n\, dt, u - u_k^*\big)\, ds_x, \quad \forall\, u \in U_{ad},$$

hence, it follows from the Lagrange calculus (Appendix B.1.2) that the optimality condition is given by

$$\int_\Gamma \big(\alpha\, u_k^* - \frac{1}{\Delta t}\int_{t_{k-1}}^{t_k} T\cdot n\, dt, u - u_k^*\big)\, ds_x \geq 0, \quad \forall\, u \in U_{ad}. \tag{5.13}$$

In summary, the necessary optimality system is given by the equality constraints (4.39) for (v,c,w), the adjoint system (5.10) for (π,ξ,η) and the optimality condition (5.13) for u^*.

5.2.1 An Apriori Bound for Galerkin Solutions of the Adjoint System

In this section we prove the existence of solutions to the adjoint system (5.10). Since the adjoint system(5.10) is a linear system of equations for $p=(\pi,\xi,\eta)$, we establish an apriori bound of the Galerkin solutions, and then by Mazurs Lemma, we extract the convex combination that converges strongly to the weak limit. Thus, the weak limit satisfies the adjoint system (5.10). To establish an apriori bound for the Galerkin solutions $\pi=\pi^n, \xi=\xi^n, \eta=\eta^n$ as in (4.45) of the adjoint system (5.10), we apply the test functions $\phi=\pi, \psi_1=\xi, \psi_2=\xi$ to (5.10) as

$$\begin{cases} -(\frac{d}{dt}\pi,\pi) + b(\pi,v,\pi) + b(v,\pi,\pi) + \mu(\nabla\pi,\nabla\pi) - (c\,\pi,\nabla\xi) + (v - v_d,\pi) = 0, \\[2ex] -(\frac{d}{dt}\xi,\xi) - (\xi\, v,\nabla\xi) - (w\nabla\xi,\pi) + (\nabla\xi,\nabla\eta) + (F''(c)\xi,\eta) + (c - c_d,\xi) = 0, \\[2ex] -(\eta,\xi) - (\xi\nabla c,\pi) + (\nabla\xi,\nabla\xi) = 0, \\[2ex] \pi(T) = 0, \;\; \xi(T) = 0. \end{cases} \tag{5.14}$$

Add the first and third equations in (5.14) together,

$$-(\frac{d}{dt}\pi,\pi) + b(\pi,v,\pi) + \mu(\nabla\pi,\nabla\pi) - (\eta,\xi) + (\nabla\xi,\nabla\xi) + (v - v_d,\pi) = 0, \tag{5.15}$$

since $b(v,\pi,\pi)=0$. Note that the terms $(c\,\pi,\nabla\xi)$ and $(\xi\nabla c,\pi)$ cancels out, since

$$(c\,\nabla\xi + \xi\nabla c,\pi) = (\nabla(c\,\xi),\pi) = 0, \quad \text{since } \; n\cdot\pi = 0, \text{ and } \operatorname{div}\pi = 0.$$

Now, integrate (5.15) backward in time

$$\frac{1}{2}(\pi(t),\pi(T))_{H_0} + \int_t^T \big(b(\pi,v,\pi) + \mu(\nabla\pi,\nabla\pi) - (\eta,\xi) + (\nabla\xi,\nabla\xi) + (v - v_d,\pi)\big)\,dt = 0. \quad (5.16)$$

Next, let $\psi_2 = -\eta$, then the third equation in (5.10) becomes

$$(\eta,\eta) + (\eta\cdot\nabla c,\pi) - (\nabla\xi,\nabla\eta) = 0. \quad (5.17)$$

Summing up (5.17) and the second equation in (5.14), we get

$$-(\frac{d}{dt}\xi,\xi) - (\xi\,v,\nabla\xi) - (w\nabla\xi,\pi) + (F''(c)\xi,\eta) + (\eta,\eta) + (\eta\cdot\nabla c,\pi) + (c - c_d,\xi) = 0. \quad (5.18)$$

Integrating (5.18) backward in time, we get

$$\frac{1}{2}(\xi(t),\xi(T))_{L^2} + \int_t^T \big(-(\xi\,v,\nabla\xi) - (w\nabla\xi,\pi) + (F''(c)\xi,\eta) + (\eta,\eta) + (\eta\cdot\nabla c,\pi) + (c - c_d,\xi)\big)\,dt = 0. \quad (5.19)$$

Now, we will estimates the terms in the weak form of the adjoint system. Starting with

$$|b(\pi,v,\pi)| \le M\,|v|_V\;|\pi|_{V_0}^{1/2}\;|\pi|_{H_0}^{1/2}.$$

Next, for the term $(w\,\nabla\xi,\pi)$, consider

$$|(w\,\nabla\xi,\pi)| = |(\xi\cdot\nabla w,\pi)| \le M\;|\nabla w|_{L^2}\;|\pi|_{V_0}^{1/2}\;|\pi|_{H_0}^{1/2}\;|\xi|_{H^1}^{1/2}\;|\xi|_{L^2}^{1/2}$$

$$\le \frac{1}{\mu}\,M^2\;|\nabla w|_{L^2}^2(|\pi|_{H_0}^2 + |\xi|_{L^2}^2) + \frac{\mu}{4}|\pi|_{V_0}^2 + \frac{1}{2}|\xi|_{H^1}^2,$$

where we used that

$$(w\cdot\nabla\xi + \xi\cdot\nabla w,\pi) = 0.$$

Note that,

$$|F''| \le M$$

since F' is Lipschitz. Now, using $|\nabla c|_\infty \le M$, we have

$$|(\eta\cdot\nabla c,\pi)| \le M\;|\eta|_{L^2}\;|\pi|_{L^2} \le \frac{1}{4}|\eta|^2 + 4M^2\;|\pi|^2.$$

Next, we have
$$|(F''(c)\,\xi,\eta)| \leq \frac{1}{4}|\eta|^2 + M^2\,|\xi|^2,$$
and
$$|(\xi,\eta)| \leq \frac{1}{4}|\eta|^2 + |\xi|^2.$$
Note that the terms $(v-v_d,\pi))$ and $(c-c_d,\xi))$ do not include derivatives, and then
$$|(v-v_d,\pi))| \leq \frac{1}{2}|v-v_d|^2 + \frac{1}{2}|\pi|^2,$$
and
$$|(c-c_d,\xi))| \leq \frac{1}{2}|c-c_d|^2 + \frac{1}{2}|\xi|^2.$$
Now, from the third equation in (5.12), we have
$$\eta = -\pi\nabla c - \Delta\xi,$$
hence we can write
$$|\eta|^2 = |\Delta\xi|^2 + |\pi\cdot\nabla c|^2 + 2(\Delta\xi,\pi\cdot\nabla c) = \frac{1}{2}|\Delta\xi|^2 + \frac{1}{2}|\Delta\xi + 2\pi\cdot\nabla c|^2 - |\pi\cdot\nabla c|^2, \tag{5.20}$$
where
$$|\pi\cdot\nabla c|^2 \leq |\nabla c|^2_\infty\,|\pi|^2_{H_0}.$$
Thus, from (5.20), we have
$$|\eta|^2 \leq \frac{1}{2}|\Delta\xi|^2 + \frac{1}{2}|\Delta\xi + 2\pi\cdot\nabla c|^2 - |\nabla c|^2_\infty\,|\pi|^2_{H_0}.$$
Next, using that $\xi\in H^2(\Omega)$, we get
$$|(v\cdot\nabla\xi,\xi)| \leq |v|_H\,|\nabla\xi|_{L^2}\,|\xi|_\infty, \tag{5.21}$$
where
$$|v|_H \leq M \quad\text{and}\quad |\xi|_\infty \leq |\Delta\xi|^{1/2}_{L^2}\,|\xi|^{1/2}_{L^2}.$$
So, (5.21) becomes
$$|(v\cdot\nabla\xi,\xi)| \leq M\,|\nabla\xi|_{L^2}\,|\Delta\xi|^{1/2}_{L^2}\,|\xi|^{1/2}_{L^2},$$

which implies that

$$|(v\cdot\nabla\xi,\xi)| \le M(\mu_1|\nabla\xi|^2_{L^2} + \mu_2|\Delta\xi|_{L^2} + \frac{1}{\mu_1\,\mu_2}|\xi|_{L^2}).$$

Thus, there exists $\alpha(t)\in L^1(0,T)$ and $M>0$ such that

$$\begin{aligned} C(t) &= \frac{1}{2}\big(|\xi(t)|^2_{L^2} + |\pi(t)|^2_{H^0}\big) + \int_t^T \frac{1}{4}\big(|\nabla\xi|^2 + \mu|\pi|^2 + |\eta|^2 + |\Delta\xi|^2\big)\,ds \\ &\le \int_t^T \alpha(t)\big(|\pi|^2 + |\xi|^2\big) + M\big(|v-v_d|^2 + |c-c_d|^2\big)\,ds, \end{aligned} \tag{5.22}$$

and hence it follows from Grönwall's inequality that $C(t)$, $t\in[0,T]$ is bounded. Since the adjoint system is linear, the convergence of Galerkin approximations to solutions of the adjoint system follows from Mazur's lemma, which states that any weakly convergent sequence in a Banach space has a convex combination sequence that converges strongly to the same limit.

5.3 Numerical Methods for Cahn-Hilliard Navier-Stokes System

Our numerical method is based on discretization of the free energy of the system (4.40). That is, the derivatives can be discretized as

$$\begin{aligned} \frac{\partial c}{\partial x_1} &\sim \frac{c_{i,j}-c_{i,j-1}}{\Delta x} \\ \frac{\partial c}{\partial x_2} &\sim \frac{c_{i,j}-c_{i-1,j}}{\Delta x} \end{aligned} \tag{5.23}$$

where c_{ij} is defined at the node points $(i\Delta x, j\Delta x)$, $0\le i,j\le N$, with mesh size Δx. The discrete energy potential can be written as

$$\int_\Omega |\nabla c|^2\,dx \sim (\sum_i^{\prime\prime}\sum_{j=1}^n |\frac{c_{i,j}-c_{i,j-1}}{\Delta x}|^2 + \sum_j^{\prime\prime}\sum_{i=1}^n |\frac{c_{i,j}-c_{i-1,j}}{\Delta x}|^2)\,\Delta x^2, \tag{5.24}$$

and the discrete mass

$$\int_\Omega |c|^2\,dx \sim \sum_i^{\prime\prime}\sum_j^{\prime\prime}|c_{i,j}|^2\,\Delta x^2. \tag{5.25}$$

Define the (one-dimensional) difference matrix d as

$$d = \begin{pmatrix} -1 & 1 & 0 & \dots & 0 \\ 0 & -1 & 1 & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots & \\ 0 & \dots & 0 & -1 & 1 \end{pmatrix},$$

and the (one-dimensional) mass matrix q as

$$q = \begin{pmatrix} 1/2 & 0 & \dots & 0 \\ 0 & 1 & 0 & \vdots \\ \vdots & \ddots & \ddots & \ddots \\ 0 & \dots & 0 & 1/2 \end{pmatrix}.$$

Set $D = d'd$, and $Q = kron(q, q)$, then, the matrix representation of the Laplacian Δ_h

$$\Delta_h = Q^{-1}(kron(D, q) + kron(q, D)). \tag{5.26}$$

Now, since div $v = 0$, we can represent the conviction term $v\ \nabla c$ as

$$v\ \nabla c = (\text{div } v) \cdot c + \nabla \cdot (v\ c) = \nabla \cdot (v\ c), \tag{5.27}$$

So,

$$\int_\Omega v\ \nabla c\ dx = \int_\Omega \nabla \cdot (v\ c)\ dx \tag{5.28}$$

The discrete form of the transport term $\nabla \cdot (v\ c)$, with $v = (a, b)$ is given by

$$\frac{1}{2\Delta x} \int_{\Omega_{ij}} \nabla \cdot (a(x), b(x)) c\, dx = \frac{1}{2\Delta x} \int_{\partial\Omega_{ij}} n \cdot (a, b) c\, ds$$

$$\sim \frac{1}{6}((ac)_{i+1,j+1} + 4(ac)_{i+1,j} + (ac)_{i+1,j-1}) - \frac{1}{6}((ac)_{i-1,j+1} + 4(ac)_{i-1,j} + (ac)_{i-1,j-1})$$

$$+\frac{1}{6}((bc)_{i+1,j+1} + 4(bc)_{i,j+1} + (bc)_{i-1,j+1}) - \frac{1}{6}((bc)_{i+1,j-1} + 4(bc)_{i,j-1} + (bc)_{i-1,j-1}). \tag{5.29}$$

where we used the Simpson's rule for the line integrals, i.e.

$$\frac{1}{b-a}\int_a^b f(x)\,dx \sim \frac{f(a)+4f(\frac{a+b}{2})+f(b)}{6}. \tag{5.30}$$

Define

$$s = \begin{pmatrix} \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & \dots & 0 \\ 0 & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} & \vdots \\ \vdots & \ddots & \ddots & \ddots & \\ 0 & \dots & \frac{1}{6} & \frac{2}{3} & \frac{1}{6} \end{pmatrix}, \quad D_1 = kron(d,s) \text{ and } D_2 = kron(s,d).$$

Then, the representation for the transport term $\nabla\cdot(c\,v)$ is

$$\nabla_h\cdot(c\,v) = D_1(a\,c) + D_2(b\,c), \quad v=(a,b). \tag{5.31}$$

From the the system (4.40), we have the discrete system for $c = c_{ij}$ as

$$\begin{cases} \dfrac{d}{dt}c - \Delta_h w + \nabla_h(c\,v) = 0, & \text{in } \Omega \\ \\ -\Delta_h c + F'(c) = w, & \text{in } \Omega \end{cases} \tag{5.32}$$

In order to integrate the system (5.32) in time, first, we substitute the second equation in the first one and use the explicit-implicit scheme as

$$\frac{c^{n+1}-c^n}{\Delta t} + \alpha\,\Delta_h(\gamma\,\Delta_h c^{n+1} - F''(c^n)(c^{n+1}-c^n) + F'(c^n)) + \frac{3}{2}\nabla_h\cdot(v\,c^n) - \frac{1}{2}\nabla_h\cdot(v\,c^{n-1}) = 0, \tag{5.33}$$

where $\alpha > 0$ is the diffusion coefficient, γ is the scaling parameter. The convictive term is treated by the second order explicit scheme in time and we use the tangent equation for $F'(c^{n+1})$

$$F'(c^{n+1}) \sim F''(c^n)(c^{n+1}-c^n) + F'(c^n). \tag{5.34}$$

Thus, we have implicit scheme for the chemical potential driven term.

5.3.1 Numerics and Discretization of Navier-Stokes System

In this section we describe the discretization of Navier-Stokes system for the velocity v. Recall the incompressible Navier-Stokes equations for the velocity v

$$\begin{cases} \dfrac{d}{dt}v - \mu\,\Delta v + v\cdot\nabla v + \nabla p = w\nabla c, \\[2em] \text{div } v = 0 \end{cases} \tag{5.35}$$

with div $= -(\nabla)^*$. Let $x_{i,j} = (ih, jh)$ be the uniform Cartesian grid with mesh size $h > 0$.

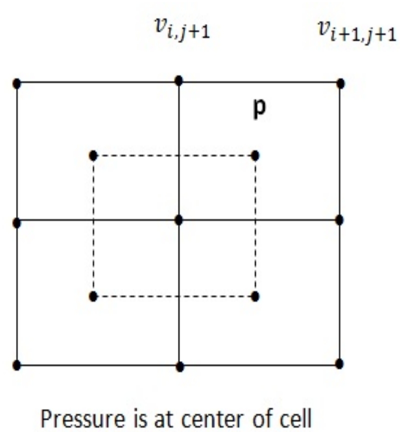

Figure 5.1 The velocity is located at the nodal points

We use the staggered grid for the pressure only, i.e., let $v_{i,j}$ be the velocity field at the grid $x_{i,j}$ and $p_{i+\frac{1}{2},j+\frac{1}{2}}$ be the pressure at the center $x_{i+\frac{1}{2},j+\frac{1}{2}} = ((i+\frac{1}{2})h, (j+\frac{1}{2})h)$ of each cell $\Omega_{i,j} = (ih, (i+1)h) \times (jh, (j+1)h)$. As shown in Figure (5.1), the velocity $v = v_{ij}$ is located at the node points $(i\,h, j\,h)$, $\;0 \le i, j \le N$. First, we develop the second order method. From the divergence condition

$$
\begin{aligned}
0 &= \int_{\Omega_{i,j}} \nabla \cdot v \, dx = \int_{\partial\Omega_{i,j}} n \cdot v \, ds_x \\
&= \int_{jh}^{(j+1)h} (v^1((i+1)h, x_2) - v^1(ih, x_2))\, dx_2 + \int_{ih}^{(i+1)h} (v^2(x_1, (j+1)h) - v^2(x_1, jh))\, dx_1
\end{aligned}
\tag{5.36}
$$

which implies that

$$
\nabla_h \cdot v = \frac{v^1_{i+1,j+1} + v^1_{i+1,j}}{2h} - \frac{v^1_{i,j+1} + v^1_{i,j}}{2h} + \frac{v^2_{i,j+1} + v^2_{i+1,j+1}}{2h} - \frac{v^2_{i+1,j} + v^2_{i,j}}{2h} = 0, \tag{5.37}
$$

where the trapezoidal rule is used for the surface integral. Note that the divergence is placed at the pressure node as we see in Figure 5.2, and note also that $\nabla_h \cdot = -(\nabla_h)^*$. Similarly, at

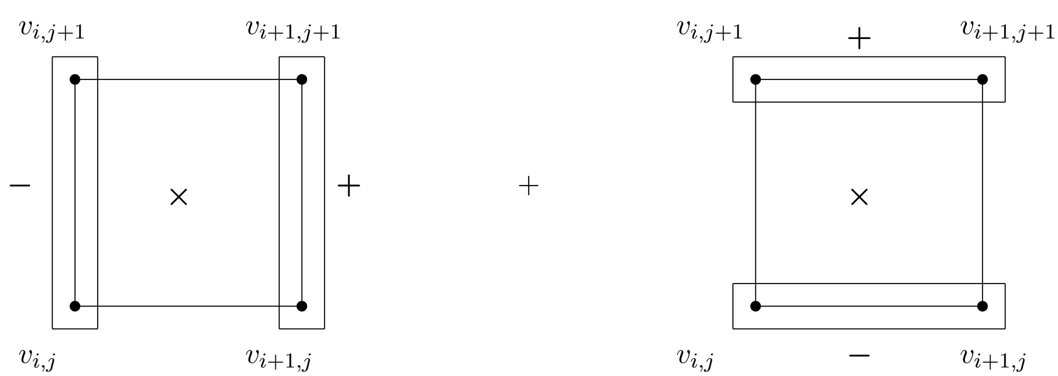

Figure 5.2 Divergence term div v located at i, j pressure node

$x_{i,j}$ we have the second order difference for the pressure gradient based on the volume integral

$$\int_{(i-1/2)h}^{(i+1/2)h} \int_{(j-1/2)h}^{(j+1/2)h} \nabla p \; dx_1 \, dx_2$$

$$= \int_{(j-1/2)h}^{(j+1/2)h} p((i+1/2)h, x_2) \; dx_2 - \int_{(j-1/2)h}^{(j+1/2)h} p((i-1/2)h, x_2) \; dx_2 \tag{5.38}$$

$$+ \int_{(i-1/2)h}^{(i+1/2)h} p(x_1, (j+1/2)h) \; dx_1 - \int_{(j-1/2)h}^{(j+1/2)h} p(x_1, (j-1/2)h) \; dx_1.$$

Using the trapezoidal rule for the surface integral, i.e

$$\int_a^b f(x) \; dx = \frac{f(b)+f(a)}{2}(b-a) + \frac{(b-a)^3}{12} f''(c), \quad c \in [a,b], \tag{5.39}$$

we obtain the second order approximation for $\nabla_h p$ as

$$\nabla_h p = \begin{pmatrix} \dfrac{p_{i+\frac{1}{2},j+\frac{1}{2}} + p_{i+\frac{1}{2},j-\frac{1}{2}}}{2h} - \dfrac{p_{i-\frac{1}{2},j+\frac{1}{2}} + p_{i-\frac{1}{2},j-\frac{1}{2}}}{2h} \\ \\ \dfrac{p_{i+\frac{1}{2},j+\frac{1}{2}} + p_{i-\frac{1}{2},j+\frac{1}{2}}}{2h} - \dfrac{p_{i-\frac{1}{2},j-\frac{1}{2}} + p_{i-\frac{1}{2},j-\frac{1}{2}}}{2h} \end{pmatrix}. \tag{5.40}$$

For the convective term $v \cdot \nabla v$ we use exactly the same discretization for the transport time as in Cahn-Hilliard equation, i.e.,

$$\frac{1}{2\Delta x} \int_{\Omega_{ij}} \nabla \cdot ((v_1, v_2)\phi) \, dx = \frac{1}{2\Delta x} \int_{\partial\Omega_{ij}} n \cdot ((v_1, v_2)\phi) \, ds \sim (v \cdot \nabla v)_h$$

$$= \frac{1}{6}((v_1\phi)_{i+1,j+1} + 4(v_1\phi)_{i+1,j} + (v_1\phi)_{i+1,j-1}) - \frac{1}{6}((v_1\phi)_{i-1,j+1} + 4(v_1\phi)_{i-1,j} + (v_1\phi)_{i-1,j-1})$$

$$+\frac{1}{6}((v_2\phi)_{i+1,j+1} + 4(v_2\phi)_{i,j+1} + (v_2\phi)_{i-1,j+1}) - \frac{1}{6}((v_2\phi)_{i+1,j-1} + 4(v_2\phi)_{i,j-1} + (v_2\phi)_{i-1,j-1}),$$

for $\phi = v_1,\ v_2$, respectively. Thus, given current velocity v^n and current pressure p^n as well as previous velocity v^{n-1}, we update v^{n+1} and p^{n+1} by solving the scheme

$$\begin{cases} \dfrac{v^{n+1}-v^n}{\Delta t} + \mu\, \Delta_h(\dfrac{v^{n+1}+v^n}{2}) + \dfrac{3}{2}(v^n \cdot \nabla_h v^n) - \dfrac{1}{2}(v^{n-1} \cdot \nabla_h v^{n-1}) + \nabla_h\, p^{n+1} = w^{n+1} \nabla c^{n+1}, \\ \\ \nabla_h \cdot\, v^{n+1} = 0. \end{cases} \tag{5.41}$$

Here, we used the Crank-Nicklson method for the Stokes term, and for the convictive term again we use the second order explicit scheme in time.

5.3.1.1 Numerical Test Examples

In this section we provide the MATLAB implementation for the Cahn-Hilliard equations with given rotation vector field $\vec{v} = (0.5 - y, x - 0.5)$. Here we use
$n = 200, dt = 0.1, dx = 0.05, \alpha = 1e-3, \varepsilon = 2e-4, \beta = .02, \lambda = 0.1.$

The results of this test are shown in Figure (5.3) below. The full MATLAB code is given as

```
n=200; e=ones(n,1);  d=n*spdiags([-e e],[0 1],n,n+1);  D=d'*d; m=n+1; dt=0.1;
q=speye(n+1); q(1,1)=.5; q(n+1,n+1)=.5; D=kron(q,D)+kron(D,q);
q=kron(q,q); DD=D*(q\D); dx=1/n; [x y]=meshgrid([0:dx:1]);
v0=1.5*cos(8*pi*x).*cos(8*pi*y);
e=ones(n+1,1); s=spdiags([-e e],[0 2],n+1,n+3);
ss=spdiags([e 4*e e]/6,0:2,n+1,n+3); %% q=kron(ss,ss);
s1=kron(s,ss); s2=kron(ss,s); s1=s1/2; s2=s2/2;
v0=v0(:); vv=zeros(n+3,n+3);  v=v0; %% q=kron(ss,ss);
[x0 y0]=meshgrid(-dx:dx:1+dx); a=.5-y0; b=x0-.5;
al=1e-3; ep=2e-4; bt=.02; lmd=0.1; v=v0(:); for k=1:20;
u=reshape(v,n+1,n+1); vv(2:n+2,2:n+2)=u;
vv(2:n+2,1)=u(:,1); vv(2:n+2,end)=u(:,end);
vv(1,2:n+2)=u(1,:); vv(end,2:n+2)=u(end,:); if k>1; o=w; end;
w=-lmd*(s1*(a(:).*vv(:))+s2*(b(:).*vv(:))); if k==1; o=w; end; s=1.5*w-.5*o;
u=v; dd=-20*ones((n+1)^2,1); f=0*v; k=find(v<=-1+ep);
j=find(v>=1-ep); dd(k)=1e5; dd(j)=1e5; f(k)=-1.e5; f(j)=1.e5;
v=(q+al*(dt*D*spdiags(dd,0,(n+1)^2,(n+1)^2)+dt*bt*DD))\(q*u+al*dt*D*f+q*s); end
```

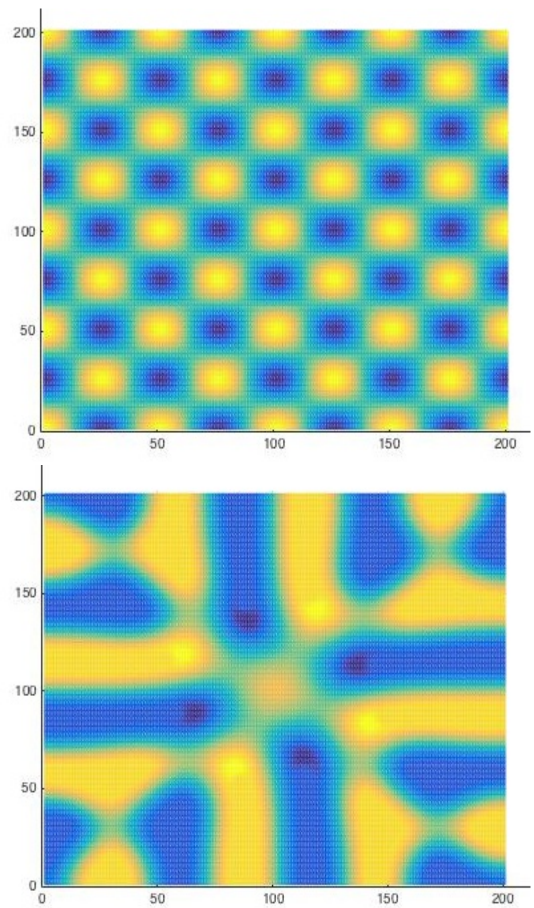

Figure 5.3 The initial and result states

Chapter 6

Summary and Conclusion

In Chapter 2 we focued on the solidification problem. We developed the variational formulation of enthalpy equation with boundary control, based on the thermal energy for the two phase Stefan problem and the corresponding weak form of equations. We showed the existence of weak enthalpy solutions by establishing an apriori bound for the weak solutions with the help of Aubin's lemma. We proved the Lipschitz continuity of solutions with respect to boundary control and initial conditions.

In Chapter 3 we formulated the optimal boundary control problem of tracking the desired motion for the solidification interface. We showed the existence of optimal control by proving the weak continuity of equality constraints. We defined the Lagrangian functional and obtained the strong form of the adjoint equation. Then we derived the necessary optimality using the Lagrange calculus. We also developed numerical discretization method with control to construct the optimal boundary control based on the sequential programing for the necessary optimality condition. Also, we presented some numerical test examples for achieving a desired solidification.

In Chapter 4 we studied the Cahn-Hiiliard Navier-Stokes equations. We developed the variational formulation of the Cahn-Hiiliard Navier-Stokes control system, based on the free energy formational and the corresponding weak form of equations. We proved the existence of weak solutions by establishing an apriori bound for the weak solutions using Aubin's lemma. We also proved the Lipschitz continuity of solutions with respect to velocity control and initial conditions using the Galerkin approach and Aubin's lemma for the compactness of Galerkin solutions. We used semi-group theory to lift regularity of concentration c. Also, we considered the sharpened Ginzburg-Landau potential as a specific model for our analysis and numerics. We obtained the chemical potential for the obstacle potential, i.e. the concentration c is constrained to $|c| \leq 1$, for the phase separation in terms of the L^2-multiplier and the complementary condition.

In Chapter 5 we formulated the optimal boundary control problem of tracking a desired state. We showed the existence of optimal control by proving the weak continuity of equality constraints. We obtained the adjoint system and proved the existence of Galerkin solutions to the adjoint system. We derived the necessary optimality using Lagrange calculus. We also developed numerical methods with control to construct the optimal boundary control.

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APPENDICES

Appendix A

Optimization Theory

The objective in optimization theory is to discuss the treatment of a general class of nonlinear variational problems of the form

$$\min_{y \in Y,\, u \in U} \quad J(y,u), \qquad \text{subject to} \quad E(y,u) = 0,\ G(y,u) \in \mathcal{C}, \tag{A.1}$$

where $J : Y \times U \to \mathbb{R}$ is the cost functional, $y \in Y$ is called the state, $u \in U$ is control or design parameter, and $E : Y \times U \to W$ and $G : Y \times U \to Z$ are functionals describing equality and inequality constraints. Here Y, U, W and Z are Banach spaces and $\mathcal{C}$ is a closed convex set in Z. The main issues that scientists usually consider about problem (A.1) include [47]: the existence of minimizers, optimality condition, Lagrange multiplier theory and sensitivity analysis of solutions to problem (A.1).

If we can use E to write the state variable y as a function of control u, i.e. $y = \Psi(u)$, then (A.1) becomes

$$\min_{u \in U} \ \ell(u) = J(\Psi(u), u), \qquad \text{subject to} \quad G(\Psi(u), u) \in \mathcal{C}. \tag{A.2}$$

In general, if y and u are independent variables satisfying $E(y,u) = 0$, then we can introduce a new variable $x = (y,u)$ in $X = Y \times U$, and hence, (A.1) becomes

$$\min_{x \in X} \quad J(x), \qquad \text{subject to} \quad E(x) = 0,\ G(x) \in \mathcal{C}. \tag{A.3}$$

An important class of constrained optimizations is the control form given as

$$\min \quad F(y) + H(u), \qquad \text{subject to} \quad E(y,u) = 0, \quad u \in \mathcal{C}, \tag{A.4}$$

where $\mathcal{C}$ is a closed convex subset of U. Here F and H are not necessarily continuously differentiable. Given $u \in \mathcal{C}$, we often assume that the equation $E(y, u) = 0$ has a unique solution $y = y(u) \in Y$.

A.1 Existence of Minimizers

Consider the unconstrained form of problem (A.3), i.e.

$$\min \quad J(x) \qquad \text{over} \quad x \in \mathcal{C}. \tag{A.5}$$

Assume that $\mathcal{C}$ is compact and J is lower semicontinuous. Then using the Weierstrass theorem in Banach spaces [71], problem (A.5) has a minimizer $x^* \in \mathcal{C}$. In general, we assume that J is weakly sequentially lower semicontinuous, i.e.

$$J(x) \leq \lim_{n\to\infty} \inf J(x_n),$$

for all weakly convergent sequences $x_n \to x \in X$. Furthermore, assume that J is coercive on $\mathcal{C}$, i.e.

$$J(x) \to \infty \quad \text{as} \quad |x| \to \infty,\, x \in \mathcal{C}.$$

In fact, let $\eta = \inf\limits_{x \in \mathcal{C}} J(x)$ and $x_n \in \mathcal{C}$ be a minimizing sequence, i.e., $J(x_n)$ is decreasing and $\lim_{n\to\infty} J(x_n) = \eta$. If X is reflexive, then there exists a weakly convergent subsequence (x_{n_k}) to $\bar{x} \in \mathcal{C}$, and since J is weakly lower semicontinuous

$$\eta = \lim_{n_k\to\infty} J(x_{n_k}) \geq J(\bar{x}) \geq \eta,$$

which implies that $J(\bar{x}) = \eta$, and $\bar{x}$ is a minimizer.
In the case of the constrained optimization problem (A.3) with $G(x) = x$, i.e.

$$\min \quad J(x) \qquad \text{subject to} \quad E(x) = 0, \quad x \in \mathcal{C}, \tag{A.6}$$

assume that J and E are weakly continuous, i.e. for $x_n \in \mathcal{C}$ converging weakly to $x \in \mathcal{C}$, we have

$$J(x_n) \to J(x) \quad \text{and} \quad E(x_n) \;\text{converges weakly to}\; E(x).$$

Then, we conclude that there exists minimizers to (A.7).

A.2 Lagrange Multipliers Theory and Complementarity Condition

In this section, we discuss the Lagrange multiplier theory for the constrained optimization problem (A.1), see as a reference [47]. Suppose that Y, U and W are Hilbert spaces with $Z = U$ and $G(y,u) = u$ i.e., the constraint $u \in \mathcal{C}$. Also, assume that J and E are C^1. Let J_y and J_u be the Fréchet derivatives of J with respect to y and u, respectively. Let W^* be the dual space of W and denote the duality product by $\langle \cdot, \cdot \rangle_{W^* \times W}$. Define the Lagrange functional as

$$\mathcal{L}(y,u,\lambda) = J(y,u) + \langle E(y,u), \lambda \rangle_{W \times W^*}$$

where $\lambda \in W^*$ is the Lagrange multiplier associated with the equality constraint $E(y,u) = 0$. Then, it has been proven under certain conditions that there exists a multiplier $\lambda \in W^*$, where the minimizing pair (y^*, u^*) satisfies

$$\begin{cases} \mathcal{L}_y(y^*,u^*) = J_y(y^*,u^*) + E_y(y^*,u^*)^* \, \lambda = 0, \\ \mathcal{L}_u(y^*,u^*) = \langle J_u(y^*,u^*) + E_u(y^*,u^*)^* \, \lambda, v - u \rangle_{Z^* \times Z} \geq 0, \quad \forall \, v \in \mathcal{C}, \\ \mathcal{L}_\lambda = E(y^*,u^*) = 0, \quad u^* \in \mathcal{C}, \end{cases} \tag{A.7}$$

which is a system of equations in (y^*, u^*, λ). In the case $K = Z$ the second equation of (A.7) results in the equality

$$J_y(y^*,u^*) + E_u(y^*,u^*)^* \, \lambda = 0. \tag{A.8}$$

In this case, a first possibility for solving the system (A.7) for the unknowns (y^*, u^*, λ) is the use of a direct equation solver of Newton type, for example. Here the Lagrange multiplier λ is treated as an independent variable just like y and u. Alternatively, for (y^*, u^*) satisfying $E(y^*,u^*) = 0$ and λ satisfying (A.8), the gradient of $\ell(u)$ of (A.3) can be evaluated as

$$\ell_u = J_u(y^*,u^*) + E_u(y^*,u^*)^* \, \lambda.$$

Thus the combined step of determining $y \in Y$ for given $u \in \mathcal{C}$ such that $E(y,u) = 0$ and finding $\lambda \in W^*$ satisfying $J_y(y^*,u^*) + E_u(y^*,u^*)^* \, \lambda = 0$ for $(y,u) \in Y \times U$ provides a possibility for evaluating the gradient of ℓ at u.

In optimal control of differential equations, the multiplier λ is called the adjoint state and the second equation in (A.7) is called the optimality condition. In Appendix B, we will discuss in details how to obtain the necessary optimality condition.

Lastly, if $\mathcal{C}$ is simple box constraints

$$\mathcal{C} = \{z \in Z : \phi \leq z \leq \psi\},$$

where Z is a lattice with ordering $\leq$, and ϕ, ψ are elements in Z, then the second equation of (A.7) can be written as the complementarity condition

$$\begin{aligned} &J_u(y^*, u^*) + E_u(y^*, u^*)^* \lambda + \eta = 0, \\ &\eta = \max(0, \eta + (u - \psi)) + \min(0, \eta + (u - \phi)). \end{aligned} \tag{A.9}$$

Appendix B

Lagrange Calculus

In this appendix we describe the so-called Lagrange calculus for equality constraint optimization. We discuss how to obtain the necessary optimality condition in general, and then obtain the necessary optimality condition for the case of Stefan problem and Cahn-Hilliard problem.

B.1 Necessary Optimality Condition

Consider the equality constraint optimization

$$\min \quad J(x,u) \text{ subject to } E(x,u) = 0, \ \ u \in \mathcal{C} \tag{B.1}$$

where $\mathcal{C}$ is a closed convex set in U. First we assume that equality constraint $E(x,u)$ defines a solution map $x = x(u) \in X, \ \ u \in \mathcal{C}$. Define the Lagrange functional

$$\mathcal{L}(x,u,p) = J(x,u,p) + \langle E(x,u), p \rangle$$

for $x \in X$, $p \in Y$ and $u \in U$. Second, given a pair $(\bar{x}, \bar{p})$ we assume that the adjoint equation $\mathcal{L}_x(h,u,p) = 0$ for all $h \in X$, i.e.

$$E_x(\bar{x},\bar{u})^* p + J_x(\bar{x},\bar{u}) = 0 \tag{B.2}$$

has a solution $p \in Y$.
Let $u = u(s) = \bar{u} + s\,v$, where s is a length and v is a direction. Let $x = x(s)$ be the corresponding solution to $u(s)$ in the equality constraints, with $E(\bar{x},\bar{u}) = 0$. Define the error ϵ_1 for equality

constraint E by

$$0 = \langle E(x(s), u(s)) - E(\bar{x}, \bar{u}), p\rangle = (E_x(\bar{x}, \bar{u})(x(s) - \bar{x})) + E_u(\bar{x}, \bar{u})(u(s) - \bar{u})), p)\rangle + \epsilon_1, \quad \text{(B.3)}$$

i.e.,

$$\epsilon_1 = \langle E(x(s), u(s)) - E(\bar{x}, \bar{u}), p\rangle - \langle E_x(\bar{x}, \bar{u})(x - \bar{x}) - E_u(\bar{x}, \bar{u})(u - \bar{u}), p\rangle, \quad \text{(B.4)}$$

Test the adjoint equation against $x - \bar{x}$

$$\langle E_x^*(\bar{x}, \bar{u})(x - \bar{x}), p\rangle + J_x(\bar{x}, \bar{u})(x - \bar{x}) = 0. \quad \text{(B.5)}$$

Also, define the quadratic error ϵ_2 for J

$$J(x, u) - J(\bar{x}, \bar{u}) = J_x(\bar{x}, \bar{u})(x - \bar{x}) + J_u(\bar{x}, \bar{u})(u - \bar{u}) + \epsilon_2, \quad \text{(B.6)}$$

i.e.,

$$\epsilon_2 = J(x, u) - J(\bar{x}, \bar{u}) - J_x(\bar{x}, \bar{u}) - J_u(\bar{x}, \bar{u})(u - \bar{u}). \quad \text{(B.7)}$$

Assume the condition that

$$\epsilon_1 + \epsilon_2 = \mathcal{L}(x(s), u(s)) - \mathcal{L}(\bar{x}, \bar{u}) - \mathcal{L}_x(\bar{x}, \bar{u})(x(s) - \bar{x}) - \mathcal{L}_u(\bar{x}, \bar{u})(u(s) - \bar{u}) \quad \text{(B.8)}$$

Now, add up equations (B.3) and (B.6)

$$J(x,u) - J(\bar{x},\bar{u}) - J_x(\bar{x},\bar{u})(x-\bar{x}) - J_u(\bar{x},\bar{u})(u-\bar{u}) + (E_x(\bar{x},\bar{u})(x-\bar{x}) + E_u(\bar{x},\bar{u})(u-\bar{u}), p) + (\epsilon_1+\epsilon_2). \quad \text{(B.9)}$$

Using the adjoint equation (B.5), then equation (B.9) can be written as

$$J(x, u) - J(\bar{x}, \bar{u}) = (J_u(\bar{x}, \bar{u}) + E_u^*(\bar{x}, \bar{u})p, (u - \bar{u})) + (\epsilon_1 + \epsilon_2). \quad \text{(B.10)}$$

for all direction $v = u - \bar{u}$.
Now, using $\epsilon_1 + \epsilon_2 \to o(s)$, i.e. $\big(\frac{o(s)}{s} \to 0\big)$, we have

$$\lim_{s\to 0} \frac{J(x(s), u(s)) - J(\bar{x}, \bar{u})}{s} = (J_u(\bar{x}, \bar{u}) + E_u^*(\bar{x}, \bar{u})p, v) = \mathcal{L}_u(\bar{x}, \bar{x})(v) \quad \text{(B.11)}$$

Thus, suppose $(\bar{x}, \bar{u})$ is a minimizer pair of (B.1), we obtain the optimality condition

$$(J_u(\bar{x}, \bar{u}) + E_u^*(\bar{x}, \bar{u})p, u - \bar{u}) \text{ for all } u \in \mathcal{C}. \quad \text{(B.12)}$$

In summary we have the necessary optimality system

$$\begin{cases} E(\bar{x},\bar{u})=0, \\ \\ E_x(\bar{x},\bar{u})^*p+J_x(\bar{x},\bar{u}), \\ \\ (J_u(\bar{x},\bar{u})+E_u^*(\bar{x},\bar{u})p,u-\bar{u}) \text{ for all } u\in\mathcal{C}. \end{cases} \tag{B.13}$$

B.1.1 Stefan Problem Case

Recall the Lagrange functional introduced in section (3.2) for the enthalpy constraint (2.4)

$$\mathcal{L}(E,g,p)=J(E,g)+\int_0^T \big(-\kappa(\nabla\beta(E),\nabla p)+(g,p)_{\Gamma_c}-(\frac{dE}{dt},p)\big)\,dt. \tag{B.14}$$

In this case the optimality condition for g^* is given by

$$\mathcal{L}_g(E,g,p)=\alpha g^*+p=0,\ \text{ at } \Gamma_c, \tag{B.15}$$

where p satisfies the adjoint equation (3.6)

$$-\frac{dp}{dt}=\kappa\,\beta'(E)\Delta p+\Psi'(E),\quad \frac{\partial p}{\partial\nu}=0,\quad p(T)=\gamma\,\Psi'(E(T)).$$

The condition (B.8) holds since $g\to E(g)$ is Lipschitz continous as shown in Section (2.5).

B.1.2 Cahn-Hilliard Navier-Stokes Case

Recall the Lagrange functional introduced in section (5.2) for the Cahn-Hilliard Navier-Stokes control problem (4.40)

$$\begin{aligned} &\mathcal{L}(y,u,p)=J(v,c,u)+\int_0^T\langle\frac{dv}{dt},\pi\rangle+b(v,v,\pi)+\mu(\nabla v,\nabla\pi)-(w\nabla c,\pi) \\ &+\langle\frac{dc}{dt},\xi\rangle+(c\,v-\nabla w,\nabla\xi) \\ &+(w,\eta)-(\nabla c,\nabla\eta)-(F'(c),\eta) \end{aligned} \tag{B.16}$$

for $y = (v, c, w)$ and $p = (\pi, \xi, \eta)$. In this case the optimality condition for u^* is given by

$$\mathcal{L}_u(y, u, p) = \alpha u^* + T \cdot n = 0, \tag{B.17}$$

where T is the stress tensor for the adjoint equation for π

$$T = \mu\,(\nabla\pi + (\nabla\pi)^t) + q\,I,$$

and q is pressure for the first equation in the adjoint system (5.10).

Appendix C

Incompressible Navier-Stokes Equations

In this Appendix we present some useful subjects to study the incompressible Navier-Stokes equations. We begin by introducing Leray Projection of f on the spaces H_0 and H. Then we explain and apply Hodge-Decomposition theorem.

C.1 Leray Projection of f on H_0 and H

Recall that $\overline{V_0} = H_0 = \{v \in L^2(\Omega)^d : \text{div } v = 0 \text{ and } n \cdot v = 0\}$. From Hodge-Decomposition, f can be written as

$$f = \vec{u} + \nabla p, \tag{C.1}$$

with div $\vec{u} = 0$.
Apply (div) operator in both sides of equation (C.1),

$$\text{div } f = \text{div } \vec{u} + \text{div } \nabla p \Rightarrow \text{div } f = \text{div } \nabla p$$

Similarly, take normal direction in both sides of equation (C.1),

$$n \cdot f = n \cdot \vec{u} + n \cdot \nabla p \Rightarrow n \cdot f = n \cdot \nabla p$$

So, we have

$$\begin{aligned} \text{div } f &= \text{div } \nabla p \\ n \cdot f &= n \cdot \nabla p, \end{aligned}$$

which can be written in a weak form as

$$(\text{div } f, \phi) = (\nabla p, \nabla \phi) \ \forall \ \phi \in H_0^1(\Omega)$$

Now, to project f on the space $\overline{V} = H = \{v \in L^2(\Omega)^d : \text{div } v = 0 \text{ and } \int_\Gamma \vec{n} \cdot \vec{v} \, ds = 0\}$, apply (div) operator in both sides of equation (C.1),

$$\text{div } f = \text{div } \vec{u} + \text{div } \nabla p \Rightarrow \text{div } f = \text{div } \nabla p$$

Similarly, take normal direction in both sides of equation (C.1),

$$n \cdot f = n \cdot \vec{u} + n \cdot \nabla p$$

So, we have

$$\begin{aligned} \text{div } f &= \text{div } \nabla p \\ n \cdot f &= n \cdot \vec{u} + n \cdot \nabla p, \end{aligned}$$

$\Rightarrow$ div$f = \Delta p$, and $p|_\Gamma = 0$, which can be written in a weak form as

$$(\text{div } f, \phi) = (\nabla p, \nabla \phi) \ \forall \ \phi \in H_0^1(\Omega)$$

So, one can show that $\mathbb{P}\Delta =$ stokes operator, generates an analytic semigroup on H_0 (or H).

C.2 Hodge-Decomposition

Hodge-Decomposition theorem states that every vector field can be uniquely decomposed into the sum of a gradient field and a divergence-free vector field, i.e., given a vector field f on a domain Ω, then there exists a scalar function p and a vector field w such that

$$f = \nabla p + w \tag{C.2}$$

where div $w = 0$, and $n \cdot w = 0$ on the boundary $\partial\Omega$. Moreover, the gradient field ∇p and the vector field w are orthogonal in the L^2 sense, i.e.

$$\int_\Omega \nabla p \cdot q \, dx = 0. \tag{C.3}$$

Since w is divergence-free, if we take the divergence of both sides of the decomposition (C.2), we obtain

$$\begin{cases} \operatorname{div} f = \Delta p, \\ \\ \dfrac{\partial p}{\partial \nu} = n \cdot \nabla p = n \cdot f, \qquad \text{on } \partial\Omega. \end{cases} \tag{C.4}$$

This boundary value problem (C.4) has a uniqe solution p (up to an additive constant) provided that

$$\int_{\Omega} \operatorname{div} f \; dx = \int_{\partial\Omega} n \cdot f \; ds.$$

The Hodge decomposition (C.2) is a very useful tool for the analysis of the incompressible Navier-Stokes equations, since it allows us to eliminate the pressure term ∇p when we introduce the weak form of the Navier-Stokes equation.

Appendix D

Numerical Methods

In this Appendix, we describe the numerical methods that we have implemented for the Stefan problem and the Cahn-Hilliard Navier-Stokes system. First, we introduce the semi-smooth Newton's method and show the relation between the primal-dual active set method and the semi-smooth Newton's method. Then we introduce the Sequential Programing algorithm for the optimal control problems. Lastly, we explain the Conjugate Gradient method applied to Sequential Programing.

D.1 Semi-smooth Newton's Method

In this section we introduce the semi-smooth Newton's method for solving nonlinear and non-smooth equations. First, we recall the primal-dual active set method for solving variational inequalities of the form

$$\begin{cases} \min \dfrac{1}{2}a(y,y) - (f,y) \\ \\ y \in H_0^1(\Omega) \\ \\ y \leq \psi \ \text{ a.e in } \Omega, \end{cases} \tag{D.1}$$

where $a(\cdot,\cdot)$ is a coercive bilinear form on $H_0^1(\Omega) \times H_0^1(\Omega)$ and $(\cdot,\cdot)$ denotes the inner product in $L^2(\Omega)$. Let y^* denote the solution to (D.1) and let λ^* be the associated Lagrange multiplier.

The optimality system for problem (D.1) is given by

$$\begin{cases} a(y^*, v) + (\lambda^*, v) = (f, v), \quad \text{for all } \ v \in H_0^1(\Omega), \\ \\ \lambda^* = \max(0, \lambda^* + c(y^* - \psi)), \end{cases} \tag{D.2}$$

for each $c > 0$ and max is the pointwise almost everywhere maximum operation. The primal-dual active set strategy is given based on the second condition in (D.1) as the following iterative method:

Given a current pair (y_k, λ_k) of primal and dual variables:

1. Initialize $c > 0$, (y_0, λ_0), set $k = 0$.
2. Define the active set $\mathcal{A}_{k+1}$ as

$$\mathcal{A}_{k+1} = \{x : \lambda_k(x) + c(y_k(x) - \psi(x)) > 0\}, \tag{D.3}$$

and hence the inactive set $\mathcal{I}_{k+1}$ will be $\Omega \setminus \mathcal{A}_{k+1}$.

3. Solve for y_{k+1}=argmin$\{\frac{1}{2}a(y, y) - (f, y) : y = \psi$ on $\mathcal{A}_{k+1}\}$.
4. Let λ_{k+1} be the Lagrange multiplier associated to the constraint in Step 3 with $\lambda_{k+1} = 0$ on $\mathcal{I}_{k+1}$.
5. Set $k = k + 1$ and goto Step 2.

The convergence of the primal-dual active set method has been studied in [40, 50]. Next, we introduce the semi-smooth Newton's method. Let X and Z be Banach spaces and let $F : D \subset X \to Z$ be a nonlinear mapping with open domain D. The mapping F is called Newton-differentiable on the open subset $U \subset D$ if there exists a family of generalized derivatives $G : U \to \mathcal{L}(X, Z)$ such that

$$\lim_{h \to 0} \frac{1}{||h||} ||F(x + h) - F(x) - G(x + h)h|| = 0, \tag{D.4}$$

for every $x \in U$. The main result asserts that if $x^* \in U$ is a solution to $F(x) = 0$ and F is Newton-differentiable in an open neighborhood U containing x^* and $\{||G(x)^{-1}|| : x \in U\}$ is bounded, then then the Newton iteration

$$x_{k+1} = x_k - G(x_k)^{-1} F(x_k), \tag{D.5}$$

converges superlinearly to x^* provided that $||x_0 - x^*||$ is sufficiently small.
Now, Consider the regularization of the second condition in (D.2) given by

$$\lambda = \max(0, \bar{\lambda} + \gamma(y - \psi)), \quad \gamma \in (0, \infty), \tag{D.6}$$

where $\bar{\lambda} \in L^2(\Omega)$. For fixed constant $\gamma > 0$, consider a semi-smooth Newton method to solve

$$\begin{cases} a(y, v) + (\lambda, v) = (f, v), \quad \text{for all } \ v \in H_0^1(\Omega), \\ \\ \lambda = \max(0, \bar{\lambda} + \gamma(y - \psi)). \end{cases} \tag{D.7}$$

The primal-dual active set method algorithm is given as follows:
1. Initialize y_0, set $k = 0$.
2. Define the active set $\mathcal{A}_{k+1}$ as

$$\mathcal{A}_{k+1} = \{x : \bar{\lambda}(x) + \gamma(y_k - \psi)(x) > 0\}, \tag{D.8}$$

and hence the inactive set $\mathcal{I}_{k+1}$ will be $\Omega \setminus \mathcal{A}_{k+1}$.
3. Solve for $y_{k+1} \in H_0^1(\Omega)$ as

$$a(y, v) + (\bar{\lambda} + \gamma(y - \psi), \chi_{\mathcal{A}_{k+1}} v) = (f, v) \quad \text{for all } \ v \in H_0^1(\Omega). \tag{D.9}$$

4. Set λ_{k+1} as

$$\lambda_{k+1} = \begin{cases} 0, & \text{on } \ \mathcal{I}_{k+1}, \\ \\ \bar{\lambda} + \gamma(y_{k+1} - \psi), & \text{on } \ \mathcal{A}_{k+1}. \end{cases} \tag{D.10}$$

5. Stop or let $k = k + 1$ and goto Step 2.
Let $A : H_0^1(\Omega) \to H^{-1}(\Omega)$ and consider the nonlinear mapping $F : H_0^1(\Omega) \times L^2(\Omega) \to H^{-1}(\Omega) \times L^2(\Omega)$ given as

$$F(y, \lambda) = \begin{pmatrix} Ay + \lambda - f \\ \\ \lambda - \max(0, \bar{\lambda} + \gamma(y - \psi)) \end{pmatrix}.$$

A generalized derivative G of F that satisfies (D.4) is given by

$$G(y_k, \lambda_k)h = \begin{pmatrix} Ah_1 + h_2 \\ \\ h_2 - \gamma\chi_{\mathcal{A}_{k+1}} h_1 \end{pmatrix}$$

where $h = (h_1, h_2) \in H_0^1(\Omega) \times L^2(\Omega)$. The resulting semi-smooth Newton update is given by

$$\begin{cases} A\,\delta y + \delta\lambda = -Ay_k - \lambda_k + f, \\ \\ \delta\lambda = -\lambda_k, \quad \text{on } \mathcal{I}_{k+1}, \\ \\ \delta\lambda - \gamma\delta y = -\lambda_k + \bar{\lambda} + \gamma(y_k - \psi), \quad \text{on } \mathcal{A}_{k+1}, \end{cases} \tag{D.11}$$

where $\delta y = y_{k+1} - y_k$ and $\delta\lambda = \lambda_{k+1} - \lambda_k$, and coincides with steps $3 - 4$ of the primal-dual active set algorithm.

D.2 Sequential Programing Method

In this section we describe how to use the so-called Sequential Programing algorithm [47, 48] for the optimal control problem (3.1) of the Stefan problem. In general, consider

$$\min \;\; J(x, u) = F(x) + H(u), \quad \text{Subject to } \; E(x, u) = 0,$$

where the equality constrain $E(x, u) = 0$ is nonlinear. The Lagrange functional is given by

$$\mathcal{L}(x, u, p) = F(x) + H(u) + \langle p, E(x, u)\rangle,$$

and the form of the adjoint equation is given by

$$F'(x) + E_x^*(x, u)\,p = 0.$$

For the Sequential Programing method, we linearize the equality constraints. Suppose that (x^n, u^n) are given, and consider

$$\min \;\; J(x, u) = F(x) + H(u),$$

subject to linearized equality constraints

$$E_x(x^n, u^n)(x - x^n) + E_u(x^n, u^n)(u - u^n) + E(x^n, u^n) = 0.$$

The adjoint equation for the linearization is

$$F'(x) + E_x^*(x^n, u^n)p = 0,$$

if we let $F(x) = \frac{1}{2}|x - x_d|^2$, then the adjoint equation can be written as

$$E_x^*(x^n, u^n)p + (x - x_d) = 0.$$

The optimality condition is given by

$$H'(u) + E_u^*(x^n, u^n)p = 0,$$

if $H(u) = \dfrac{\alpha}{2}|u|^2$, then the optimality condition is written as

$$\alpha u + E_u^*(x^n, u^n)p = 0,$$

where the unknowns are (x, u, p), given (x^n, u^n).
In summary, the equality constrain, adjoint equation and optimality condition form the following linear system

$$\begin{cases} E_x(x^n, u^n)(x - x^n) + E_u(x^n, u^n)(u - u^n) + E(x^n, u^n) = 0, \\ E_x^*(x^n, u^n)p + (x - x_d) = 0, \\ \alpha u + E_u^*(x^n, u^n)p = 0. \end{cases} \tag{D.12}$$

which can be represented as

$$\left[\begin{array}{c|c|c} E_x & 0 & E_u \\ \hline F'(x) & E_x^* & 0 \\ \hline 0 & E_u^* & \alpha \end{array}\right] \begin{bmatrix} \text{x} \\ \text{p} \\ \text{u} \end{bmatrix} = \begin{bmatrix} \text{RHS} \\ 0 \\ 0 \end{bmatrix}$$

where RHS= $E_x x^n + E_u u^n - E$.
To solve the linear system (D.12), eliminate x using u,

$$(x - x^n) + (E_x)^{-1}(E_u(u - u^n) + E(x^n, u^n)) = 0.$$

Next, solve for p,

$$E_x^*\, p + Qx = 0 \Longrightarrow p = -(E_x^*)^{-1}Qx.$$

Then, plug in the third equation

$$\alpha u + E_u^*\, p = 0 \Longrightarrow \alpha u - E_u^*\, (E_x^*)^{-1}Qx = 0.$$

So, we get

$$\alpha u + E_u^*\, (E_x^*)^{-1}Q(E_x)^{-1}E_u u = \text{RHS} \Longrightarrow \alpha u + L * u = \text{RHS}. \tag{D.13}$$

Now, for the Stefan problem case, consider the linearizing the equality constraint (3.21), i.e.

$$\frac{E_k^n - E_k^{n-1}}{\lambda} = -\kappa H(\beta'(E_k^{n-1})(E_k^n - E_k^{n-1}) + \beta(E_k^{n-1})) + Bg^n, \tag{D.14}$$

where k is for the iterate of the sequential programing and n is for the time step. Then, we can derive the discrete time adjoint equation for p_k^n using the integration by summation formula as

$$\frac{p_k^n - p_k^{n-1}}{\lambda} = -\beta(E_k^n)\; Hp_k^n + \Psi'(E_k^n). \tag{D.15}$$

Also, the optimality condition for g_k^n is given by

$$\alpha g_k^n + p_k^n = 0. \tag{D.16}$$

We solve the system of equations (D.14), (D.15) and (D.16) for (E_k^n, p_k^n, g_k^n) using the conjugate gradient method described in next Appendix D.3.

D.3 Conjugate Gradient Method Applied to Sequential Programing

We do not want to form the matrix L since it is too expensive to do so, instead we calculate RHS=b and compute $L * u$ (The action of L on u). Consider

$$\frac{dx^n}{dt} = f(x^n(t)) + Bu^n, \tag{D.17}$$

which is equivalent to (2.4)–(2.6). The linearization of (D.17) in increment form is given by

$$\begin{aligned}\frac{d(x^+ - x^n)}{dt} &= f'(x^n)(x^+ - x^n) + B(u^+ - u^n) - (\frac{dx^n}{dt} - f(x^n) - B(u^n)),\\ \Longrightarrow \frac{d(x^+ - x^n)}{dt} &= f'(x^n)(x^+ - x^n) + B(u^+ - u^n),\\ \Longrightarrow \frac{d(\delta x)}{dt} &= f'(x^n)(\delta x) + B(\delta u).\end{aligned} \tag{D.18}$$

where $F(x) = \dfrac{dx}{dt} - f(x) - Bu = 0$. Consider the cost functional of tracking form

$$J(x, u) = \int_0^T (\frac{1}{2}\ell(x) + \frac{\alpha}{2}|u|^2)\, dt, \tag{D.19}$$

or

$$J(E, g) = \int_0^T (\frac{1}{2}|E - \overline{E}|^2_{L^2(\Omega)} + \frac{\alpha}{2}|g|^2_{L^2(\Gamma)})\, dt. \tag{D.20}$$

The sequential programing is to solve the constrain optimization

$$\min\ J(x^+, u^+), \quad \text{subject to (D.18)}. \tag{D.21}$$

Define the Lagrangian functional

$$\mathcal{L}(x, u, p) = J(x^+, u^+) + \int_0^T (p, f'(x^n)(x^+ - x^n) + B(u^+ - u^n) - \frac{d}{dt}(x^+ - x^n))\, dt, \tag{D.22}$$

then

$$\mathcal{L}_{x^+}(x^+, u^+, p)(h) = 0 \Longrightarrow \int_0^T ((\ell'(x^+) + f'(x^n)^*\, p - \frac{dp}{dt}), h)\, dt = 0,$$

for all directions h, and $p(T) = 0$. So, the adjoint equation is given by

$$-\frac{dp}{dt} = f'(x^n)^* \, p + \ell'(x^+). \tag{D.23}$$

We also have

$$\mathcal{L}_{u^+}(x^+, u^+, p)(v) = 0 \Longrightarrow \int_0^T ((\alpha u^+ + B^T \, p), v) \, dt = 0,$$

for all directions v, and $p(T) = 0$. So, we get

$$\alpha u^+ + B^T \, p = 0, \tag{D.24}$$

and we need to solve for u^+.

Now, to solve (D.21), first, consider the time discretization of (D.18)

$$\frac{x_{k+1}^+ - x_k^+}{\Delta t} = f'(x_k^n) x_{k+1}^+ + B u_k^+ + f(x_k^n) - f'(x_k^n) x_k^n, \tag{D.25}$$

where n is for iterate, k is for time, and G_k is the Jacobian $f'(x_k^n)$. So

$$x_{k+1}^+ = (I - \Delta t \; G_k) \setminus [x_k^+ + \Delta t(B u_k^+ + f(x_k^n) - G_k \; x_k^n)], \tag{D.26}$$

and the adjoint equation is

$$-\frac{dp}{dt} = G^t \; p + J'(x^+) \Longrightarrow \frac{p_k - p_{k-1}}{\Delta t} = G_k^t \; p_k + Q(x^+ - \bar{x}). \tag{D.27}$$

So, equation (D.13) can be written as

$$\alpha u + B^t \; (E_x^*)^{-1} Q (E_x)^{-1} B u(t) = \text{RHS}. \tag{D.28}$$

In summary, the algorithm to solve this problem is as follows:

(1) Given control u^n, we need to compute E^n.

(2) Solve the adjoint equation

$$-\frac{dp}{dt} = f'(x^n)^* \; p + \ell'(x^n), \quad p(T) = 0.$$

(3) Solve for u^+, using that u^n is a solution of

$$\alpha u^n + B^* \; p^n = r^n = \text{residual},$$

then solve the well-posed equation

$$\alpha u^{+} + B^{*}\, p^{+} = 0.$$

where we suppose that $|r_n| >> \epsilon$.
(4) If $p = Lv = B^{*}(E_x^{*})^{-1}QE_x^{-1}Bv$, then p^{+}, is a linear function, with $p^{+} = Lv^{+}$, and $v^{+} = u^{+} - u^{n} = \delta u$ is the increment in control.
Now, consider

$$-\frac{dp^{n}}{dt} = f'(x^{n})^{*}\, p^{n} + \ell'(x^{n}), \qquad p^{n}(T) = 0.$$

$$\Longrightarrow -\frac{d(p - p^{n})}{dt} = f'(x^{n})^{*}\, (p - p^{n}) + \ell'(x^{+}) + \ell'(x^{n}),$$

Using the increment form we can write

$$-\frac{\delta p}{dt} = f'(x^{n})^{*}\, \delta p + \ell'(\delta x), \tag{D.29}$$

$$-\frac{\delta x}{dt} = f'(x^{n})^{*}\, \delta x + B\, \delta u, \tag{D.30}$$

where $\delta x = x^{+} - x^{n}$, $\delta u = v$, and $\delta p = Lv = L(\delta u)$.
Thus, we can evaluate $B^{*}\, \delta p$, and

$$\begin{cases} \alpha u^{+} + B^{*}\, p^{+} = 0, \\ \\ \alpha u^{n} + B^{*}\, p^{n} = r^{n}. \end{cases} \tag{D.31}$$

Subtracting the two equations in (D.31), we get

$$\alpha(u^{+} - u^{n}) + B^{*}\, (p^{+} - p^{n}) = -r^{n},$$

$$\Longrightarrow \alpha\delta u + B^{*}\, \delta p = -r^{n}. \tag{D.32}$$