ON AN ORDER-PARAMETER MODEL OF SOLID-SOLID PHASE TRANSITIONS

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On an Order-Parameter Model of Solid-Solid Phase Transitions

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(ABSTRACT)

We examine a model of solid-solid phase transitions that includes thermo-elastic effects and an order parameter. The model is derived as a special case of the Gurtin-Fried model posed in one space dimension with a symmetric triple-well free energy in which the relative heights of the wells vary with temperature. We examine the temperature independent case, showing existence of a unique classical solution of a regularized system of partial differential equations using semigroup theory. This is followed by numerical study of a finite element algorithm for the temperature independent model. Finally, we present computational material concerning the temperature dependent model.

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Chapter 1

Mathematical Models of Phase Transitions

1.1 Introduction

The purpose of this paper is to examine a model of solid-solid phase transitions that includes thermo-elastic effects and an order parameter. The model is derived as a special case of the Gurtin-Fried model [61] [63] posed in one space dimension with a symmetric triple-well free energy in which the relative heights of the wells vary with temperature. We examine the temperature independent case, showing existence of a unique classical solution of a regularized system of partial differential equations using semigroup theory. This is followed by numerical study of a finite elements algorithm for the temperature independent model. We present an error estimate for the algorithm and examine quantitative information. Finally, we present computational results on the temperature dependent model.

Phase transitions occur when a material undergoes a physical change from one state to another. The most common examples are the phase changes that water undergoes as it is heated. As the internal temperature of water rises, water changes from solid (ice) to liquid and then to vapor (steam). In this paper we consider models of a different type of phase transition, that of one solid phase to another solid phase.

Phases transition from one solid state to another occur when there is a rearrangement of molecules that results in a change in the material's lattice structure. For example, a phase transition occurs when the shape of the lattice changes due to mechanical strain or temperature, but the atoms maintain the same relationship with each other in the cells of the lattice. A material may have several inherent lattice configurations such as a high-temperature, high-symmetry phase and a low-temperature, low-symmetry phase. For example, Ball and James [2] give a detailed description of the transition of Indium-Thallium from a cubic configuration to a tetragonal configuration.

Shape-memory alloys undergo just such a reversible structural phase transformation. This transformation may be triggered by a change in strain or temperature. The shape-memory effect occurs when a material in its high-symmetry phase is cooled from a temperature above its transformation temperature, T_c, to a temperature below T_c. At the lower temperature the material, in its low-symmetry phase, can undergo large changes in shape that remain until the temperature is raised above T_c, at which time the material returns to the original high-symmetry phase for which there is only one possible configuration. For more information on shape-memory materials see e.g. [91].

Physical models of these phenomena remain the subject of intense research and dispute. The mathematical properties of the models are also widely studied. In this thesis we will examine one of the many models being currently considered. We will show that it is consistent with thermodynamics, prove existence and uniqueness theorems for relevant partial differential equations, develop numerical algorithms and analyze their convergence and study numerical experiments.

We organize the remainder of this paper as follows. In the remainder of this chapter we give a brief historical overview of phase transition models followed by mathematical descriptions of these models. In Chapter 2, we describe the Gurtin-Fried model in one space dimension. In our constitutive choices we specify a symmetric triple-well free energy potential in which the relative heights of the wells vary with temperature. We present the resulting partial differential equations. We then add viscosity terms to the system of equations to regularize both the temperature independent and dependent cases. In Chapter 3, an overview of operator theory, semigroup theory and initial value problems is presented. This lays the groundwork for a theorem for the local existence and uniqueness of a classical solution of the temperature independent system of equations. In Chapter 4, we present a finite element algorithm utilizing the well known Crank-Nicolson-Galerkin method for the temperature independent model. Error estimates for each time step are proved. In Chapter 5, numerical results are shown and discussed. In Chapter 6, we show numerical computations for the temperature dependent system of equations. In Chapter 7, we discuss open questions and possibilities for future work.

1.2 Historical overview of phase transition models

In this section we give a brief outline of some of the models that had the most influence on the problem studied in this paper. Most modern day models of phase transitions are based on work done modeling compressible fluids in the late nineteenth century by Gibbs [64], Maxwell [81] and van der Waals [94]. The mathematical problem that has been considered throughout the study of phase transitions is the minimization of an energy integral with a non-convex term in the integrand. In dynamical versions of these models, this gives rise to differential equations which are elliptic away from the local minima of the potential and hyperbolic otherwise. The simplest of models, Gibbs' double-well model, is obtained from minimizing an energy functional that includes a double-well energy density. The wells of the energy density represent two distinct phases or physical states. There exists a multitude of minimizers of this basic energy [65] [77], a situation which does not reflect the physical situation.

Variations in the model, such as adding a nonlocal term [9], have been used in an attempt to restrict the number of solutions. The most popular has been an added gradient term in the integrand which inhibits large changes in the density. This model was derived by Van der Waals [94] [88] and independently by Cahn and Hilliard [37] more than half a century later. The general approach to solving this problem has been to examine the asymptotic behavior of the solution [59] [82]. For the one dimensional problem, Carr, Gurtin and Slemrod [38] showed that as the coefficient of the gradient term goes to zero, the global minimizer is monotone, has a single phase transition and is unique up to reflection. Much work has been done concerning the existence of solutions and the characterization of such solutions for these models [3] [36] [54].

In 1958, Cahn and Hilliard [37] proposed a model for an isotropic system of nonlinear composition in a binary alloy. The resulting equation is a fourth-order nonlinear parabolic equation for which spatial patterns represent phase interfaces. The Cahn-Hilliard equation is the result of minimizing a potential energy functional with a non-convex term and a gradient term. Solutions of the Cahn-Hilliard equation possessing internal layers represent phase boundaries. Bates and Fife [4] showed that when the coefficient of the gradient term is very small, the initial data in the spinodal region develop into fine-grained “mush” which coarsens in slower time scales. Using inner and outer expansions, Pego [85] carried out formal asymptotic analysis of these layered solutions. Discussion of the physical aspects of the Cahn-Hilliard model, such as interfacial energies, nucleation and spinodal decomposition, may be found in many works, such as [3] [33] [34] [35] [66] [67] [86]. Some basic mathematical properties of the equation are found, among other places, in [3] [4] [38] [47] [48] [50] [52] [85] [97].

Halperin, Holenberg and Ma [66] [67] proposed a model for a pure material undergoing phase transition which introduced an order parameter, or phase field, describing the phase of the material which is coupled with temperature. The Phase Field model is a refinement of the above model by Fix [57] and Caginalp [14] which was also derived independently by Collins and Levine [45]. The main assumption of the phase field model is that the free energy is a function of an order parameter, or “phase field”, as well as the more familiar thermodynamic variable, either temperature or concentration. This energy potential reflects both bulk free-energy differences between phases and capillary effects.

The phase field model is successful in modeling phase interfaces and mushy zones [4] [53]. This model exhibits qualitative features common to solidification of a pure material such as breakdown of planar and circular interfaces to cellular structures as well as the formation of dendrites, inclusion of liquid pockets and coarsening behavior [29] [30] [31] [75] [53] [58]. The phase field model also permits supercooling to occur, a source of nonlinear instability, as well as a nonlinear stabilization mechanism involving surface tension [58] [15]. Caginalp has shown, in various distinguished limits, that various forms of the Stefan problem [89] may be recovered in which the interface is taken to be sharp, that is, modeled by a surface [14] [16] [17] [18]. Some basic mathematical properties of the equation are found, among other places, in [12] [15] [19] [22] [23] [27] [28] [39] [51] [52]. Additional numerical results for the phase field model may be found in such works as [24] [26] [41] [40] [54] [83]. Wheeler, Boettinger and McFadden [6] extended the phase field model to binary alloys. Results for this model may be found in such works as [5] [7] [8] [25] [32]. Higher order phase field models have been proposed by Caginalp and Fife [21].

In 1990, Penrose and Fife [55] proposed a more general model which encompasses the phase field model [56]. The Penrose-Fife model is based on the observation that the second law of thermodynamics postulates that the entropy functional cannot decrease along solution paths. Whereas the phase field model is usually derived from a free energy functional that is applicable only to isothermal situations, the Penrose-Fife model is thermodynamically consistent with the physical phenomena in that it satisfies criteria to ensure the phase field will take on fixed values which represent the phase, i.e. liquid or solid. The resulting system of partial differential equations proves to be more difficult than those of the phase field equations due to a nonlinear term involving the time derivative of the phase field. Zheng [98] and again with Sprekels [92] proved the existence and uniqueness of solutions in 1-D and 3-D respectively. They also discussed the asymptotic behavior of the solutions. Additional discussion of the Penrose-Fife model may be found in such works as [11] [49] [70] [72] [73] [74]. Numerical results for the Penrose-Fife model may be found in [69].

In 1994, Gurtin and Fried [61] [63] proposed a model which, in addition to describing solidification, is general enough to describe solid-solid transitions where deformational effects dominate those associated with heat and mass transport. This model is based on general balance laws, common to large classes of materials, which are carefully distinguished from constitutive equations that differentiate between particular materials. The Gurtin-Fried model, again, uses an order parameter to characterize the notion of phase. This model utilizes the Second Law of Thermodynamics to introduce a dissipation inequality. Gurtin and Fried showed that the choice of specific parameters reduces their model to the phase field model [62].

It is the Gurtin-Fried model in one space dimension that we follow in this thesis and we present this model in great detail in Chapter 2. Additional study of the Gurtin-Fried model may be found, among other places, in [10] [60] [62] [78].

1.3 Mathematical overview of phase transition models

In this section we examine some mathematical details of the models described above.

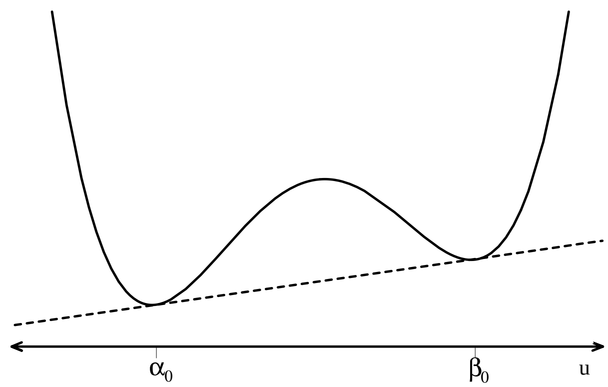

Figure 1.1: The double-well energy potential, $\mathcal{W}(u)$ (solid line), and the line $\mathcal{S}(u)$ (dashed line).

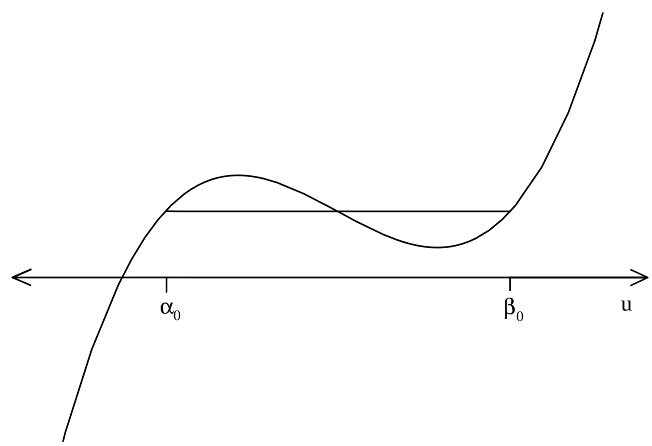

Figure 1.2: The derivatives of $\mathcal{W}(u)$ and $\mathcal{S}(u)$.

1.3.1 Gibbs' double-well model

We now examine an abstract mathematical version of Gibbs' double-well model in one space dimension. Let $\Omega = [a, b] \in \mathbb{R}$ represent a one dimensional body, a bar or rod, for example. Let $u : \mathbb{R} \to \mathbb{R}$ be some scalar quantity describing a property of the material with two natural states or phases. These physical states corresponds to local minima or wells of a potential energy $\mathcal{W} \in C^1(\mathbb{R})$ (see Figure 1.1). Phase one and phase two correspond to the local minima, u_1 and u_2, respectively. As we shall see, the section of $\mathcal{W}$ which is concave down or, rather, where $\mathcal{W}'$ is decreasing (see Figure 1.2) presents difficulties when searching for a solution to the related minimization problem. This area of the potential energy function is called the "spinodal region".

The problem to be solved is the following:

Problem 1.1 *Let $M \in \mathbb{R}$ be given. Minimize*

$$\mathcal{F}[u(\cdot)] := \int_\Omega \mathcal{W}(u(x))dx$$

over the set of $u \in L^1(\Omega)$ such that

$$\int_\Omega u(x)dx = M.$$

Necessary conditions for a piecewise continuous function, $\tilde{u}$, to be a constrained minimizer are that there exists a constant Lagrange multiplier, σ, such that $\tilde{u}$ satisfies the Euler-Lagrange equation

$$\mathcal{W}'(\tilde{u}) = \sigma \tag{1.1}$$

and $\tilde{u}$ satisfies the Weierstrass-Erdmann corner condition at points of discontinuity, that is,

$$\lim_{x \to x_0^+} \mathcal{W}(\tilde{u}(x)) - \sigma\tilde{u}(x) = \lim_{x \to x_0^-} \mathcal{W}(\tilde{u}(x)) - \sigma\tilde{u}(x) \tag{1.2}$$

where $\tilde{u}$ has a jump discontinuity at $x_0 \in [a, b]$.

We assume $\mathcal{W}$ is such that Maxwell's conditions are met, i.e., there exists a unique pair of distinct points, $\alpha_0 < \beta_0$, and a number, σ_0, such that

$$\begin{aligned} \sigma_0 &= \mathcal{W}'(\alpha_0) = \mathcal{W}'(\beta_0) \\ \mathcal{W}(\beta_0) - \mathcal{W}(\alpha_0) &= \sigma_0(\beta_0 - \alpha_0). \end{aligned}$$

We define the function $\mathcal{S}$ by

$$\mathcal{S}(u) = \sigma_0 u + \mathcal{W}(\alpha_0) - \sigma_0\alpha_0.$$

We assume that $\mathcal{S}(u) \leq \mathcal{W}(u)$ for all u (see Figure 1.1). We further assume that $u \to \mathcal{W}(u) - \mathcal{S}(u)$ has exactly two global minimizers at $u = \alpha_0, \beta_0$. Then, since $\int_\Omega \mathcal{S}(u)dx$ is constant for all $u \in L^1(\Omega)$ such that $\int_\Omega u(x)dx = M$, Problem 1.1 is equivalent to the auxiliary problem:

Problem 1.2 *Let $M \in \mathbb{R}$ be given. Minimize*

$$\mathcal{F}^*[u(\cdot)] := \int_\Omega \mathcal{W}(u(x)) - \mathcal{S}(u(x))dx = \int_\Omega \{\mathcal{W}(u(x)) - \sigma_0 u(x) + \mathcal{W}(\alpha_0) - \sigma_0\alpha_0\}dx.$$

over the set of $u \in L^1(\Omega)$ such that

$$\int_\Omega u(x)dx = M.$$

The solutions to Problem 1.2 are a class of global minimizers which are either constant (single phase) or piecewise constant (two phases). If $M \in (\alpha_0, \beta_0)$, then one can describe a class of phase solutions of the form

$$u(x) = \begin{cases} \alpha_0 & x \in S_1 \\ \beta_0 & x \in S_2, \end{cases} \tag{1.3}$$

where S_1 and S_2 are disjoint measurable sets such that $S_1 \cup S_2 = \Omega$. If $M \leq \alpha_0$ or $\beta_0 \leq M$, the solution is $u = \dfrac{M}{|\Omega|}$, the average density. For more details see e.g. [78].

1.3.2 An added gradient term

The previous model permits a large multiplicity of solutions which does not reflect physical phenomena. In order to refine Gibbs' model, a gradient term, $u_x(\cdot)$ is added to the integrand of $\mathcal{F}$.

Problem 1.3 *Minimize*

$$\mathcal{F}_\epsilon[u(\cdot)] = \int_\Omega \mathcal{W}(u(x)) + \frac{\epsilon^2}{2}|u_x(x)|^2 dx$$

over the set of $u(\cdot) \in H^1(\Omega)$ *such that*

$$\int_\Omega u(\mathbf{x})d\mathbf{x} = M.$$

here, ϵ is a small parameter. The added gradient term penalizes large changes in the density. The Euler equation is now

$$\mathcal{W}'(u(x)) - \epsilon^2 u_{xx}(x) = \sigma_0.$$

Carr, Gurtin and Slemrod [38] considered the problem of finding

$$\bar{u}(x) = \lim_{\epsilon \to 0} u_\epsilon(x).$$

for the following minimization problem.

Problem 1.4 *Let* $M \in \mathbb{R}$ *be given. Minimize*

$$\mathcal{F}[u(\cdot)] := \int_{-L}^{L} \mathcal{W}(u(x)) + \frac{\epsilon^2}{2}|u'(x)|^2 dx$$

over the set of $u \in H^1[-L, L]$ *such that*

$$\int_{-L}^{L} u(x)dx = M.$$

They showed that Problem 1.4 has a unique global minimizer, u_ϵ for all $\epsilon > 0$ and, as $\epsilon \to 0$,

$$u_\epsilon(x) \to u_0(x)$$

where u_0 is a single interface solution of the form

$$u_0(x) = \begin{cases} \alpha_0 & -L \leq x < -L + l_1 \\ \beta_0 & -L + l_1 \leq x \leq L. \end{cases}$$

Modica [82] and Fonseca and Tartar [59] showed existence of solutions in $\mathbb{R}^n, n \geq 2$ and convergence for small ϵ in $L^2(\Omega)$ using compactness results.

1.3.3 Non-local model

Brandon, Lin and Rogers [9] introduced a non-local functional for the phase transition problem based on similar models in ferromagnetism in $1 - D$. They define the energy functional $\mathcal{F}$ as follows:

$$\mathcal{F}[u] = \int_{-1}^{1} \mathcal{W}^{**}(u(x))dx - \frac{1}{2}\int_{-1}^{1}\int_{-1}^{1} k(x,y)u(x)u(y)dxdy$$

where

$$\mathcal{W}^{**}(u) = \begin{cases} \mathcal{W}(u) & u \leq \alpha_0 \\ \mathcal{S}(u) & \alpha_0 < u < \beta_0 \\ \mathcal{W}(u) & \beta_0 \leq u \end{cases}$$

is the convex hull of $\mathcal{W}$, k is a symmetric kernel and the operator

$$g[u](\cdot) := \int_{-1}^{1} k(\cdot, y)u(y)dy$$

is compact. In addition to an existence result, it was also shown that, for special kernels, this model is equivalent to that of the static configurational model proposed by Gurtin and Fried [61] [63] as a minimization problem:

Problem 1.5 *Minimize*

$$\begin{aligned} \mathcal{F}[u,\phi] &= \int_{-1}^{1} \mathcal{W}^{**}(u) + c(\frac{1}{2}\phi^2 + \phi u) + \frac{\epsilon^2}{2}|\phi'|^2 dx \\ &\quad + \frac{\epsilon^2}{2}\gamma(|\phi(1)|^2 + |\phi(-1)|^2) \end{aligned}$$

over the set of all (u,ϕ) *such that*

$$\int_{-L}^{L} u(x)dx = M.$$

Here ϕ is an order parameter. We note that Gurtin and Fried did not present their model as the result of a minimization problem. However, their equations in the static case are the result of a minimization problem.

1.3.4 The Cahn-Hilliard model

Cahn and Hilliard [36] [37] use the functional

$$\mathcal{F}[u(x,t)] = \int_{\Omega} \mathcal{W}(u(x,t)) + \frac{\epsilon^2}{2}|\nabla u(x,t)|^2 dx$$

to derive an equation which models the dynamical behavior of a binary material. The equation

$$u_t(x,t) = m\Delta[\mathcal{W}'(u(x,t)) - \epsilon^2 \Delta u(x,t)]$$

is known as the Cahn-Hilliard equation. The variable $u(x,t)$ measures the concentration of a solute in a pure material or the density of one component of an alloy. The energy density $\mathcal{W}(u)$ is the Helmholz free energy of a unit volume of homogeneous material of composition u. The mass of the material is assumed to remain constant, hence the constraint

$$\int_{\Omega} u(x,t)dx = M \quad t \in [t_0, t_1].$$

For problems in one space dimension, Bates and Fife [3] show the existence of a spike-like stationary, yet unstable, solution which they call a canonical nucleus. Solutions of the Cahn-Hilliard equation possessing internal layers represent phase boundaries. Bates and Fife [4] showed that when the coefficient of the gradient term goes to zero, the initial data in the spinodal region develop into fine-grained “mush” which coarsens in slower time scales. Pego, [85], carried out formal asymptotic analysis of these layered solutions using inner and outer expansions. The Cahn-Hilliard equation models physical aspects of binary alloys, such as interfacial energies, nucleation and spinodal decomposition [3] [33] [34] [35] [66] [67] [86]. Discussion of the mathematical properties of the model are found, among other places, in [3] [4] [38] [47] [48] [50] [52] [85] [97].

1.3.5 The phase field model

The phase field model uses a continuous order parameter, ϕ, to describes a pure material undergoing a phase transition. Temperature, θ, which has been assumed constant in the previous discussion, is now allowed to vary. The functional used in the phase field models take the general form:

$$\mathcal{F}[\phi,\theta] = \int_{\Omega} g(\phi,\theta) + f(\nabla\phi)dx.$$

Halperin, Holenberg and Ma [66] [67] introduced the use of general energy functionals as a means of considering the dynamic critical phenomena. These general models were refined by Fix [57] and Caginalp [14]. It was also independently derived by Collins and Levine [45] using the functional

$$\mathcal{F}[\phi,\theta] = \int_{\Omega} \{\alpha|\nabla\phi|^2 + \beta(\phi^2-1)^2 + c\theta\phi\}dx. \tag{1.4}$$

The phase field equations used by Caginalp [14] are given by the Euler-Lagrange derivative of $\mathcal{F}$ coupled with the heat equation:

$$\begin{aligned}\tau\phi_t = \frac{\partial \mathcal{F}}{\partial \phi} &= \phi^3 - \phi - \epsilon^2 \Delta\phi + 2\theta \\ \theta_t - \frac{1}{2}\phi_t &= m\Delta\theta.\end{aligned}$$

Here the constants from (1.4) are $\alpha = \frac{1}{2}\epsilon^2, \beta = \frac{1}{4}$ and $c = 2$. The constant, τ, is the relaxation parameter (in time).

Caginalp, along with others, has studied the phase field model extensively. Topics studied by Caginalp include existence, uniqueness and the regularity of solution [14] (with Fife) [22] (with Nishiura) [27], ODE's resulting from the static model (with Hastings) [24], numerical analysis of the behavior of the phase boundary (with Lin) [26], phase field model as the general case of the Stefan, Hele-Shaw and Cahn-Hilliard models [16] [17] [18](with Fife) [28] (with Chen) [20], numerical studies of phase field equations in $\mathbb{R}$ and $\mathbb{R}^2$ and $\mathbb{R}^n$ with radial symmetry (with Socolovsky) [29] [30] [31], and higher order phase field models [15] (with Fife) [21]. Other studies of the phase field model may be found in [11] [12] [39] [40] [41] [49] [53] [54] [58] [75] [76] [83].

The phase field model has been extended to the solidification of a binary material. One such model by Caginalp and Xie [32] is based on the free energy functional:

$$\mathcal{F}[\phi, \theta, c] = \int_\Omega f(c)|\nabla\phi|^2 + g(\phi, \theta, c)dx$$

where $c(x,t)$ represents the concentration of one of the components of the alloy. The resulting phase field equations are:

$$\begin{aligned}\tau_1\phi_t &= \frac{\partial \mathcal{F}}{\partial \phi} \\ c_v\theta_t - \nabla \cdot k_1 \nabla\theta &= H(\phi, c, \phi_t, c_t) \\ \tau_2 c_t &= \nabla \cdot k_2 c(1-c)\nabla(\frac{\partial \mathcal{F}}{\partial c})\end{aligned}$$

Other models of this type have been introduced by Wheeler, Boettinger, McFadden [6] [7], and with Murray and Kobayashi [5].

1.3.6 The Penrose-Fife model

Penrose and Fife [55] [56] proposed an alternative order parameter model for phase transition based on the Second Law of Thermodynamics in terms of entropy. The entropy functional used is

$$\mathcal{F}[e, \phi] = \int_\Omega S(e, \phi) - \frac{1}{2}k|\nabla\phi|^2 dx$$

where $\phi(x,t)$ is an order parameter, $e(x,t)$ is the energy density and $S(e,\phi)$ is the entropy density. The relationship between the energy density and temperature, θ, is given by

$$e = \frac{\partial\left(\frac{f(\theta,\phi)}{\theta}\right)}{\partial\left(\frac{1}{\theta}\right)}$$

where $f(\theta,\phi)$ is the free energy density.

The dynamic equations of the Penrose-Fife model are

$$\begin{aligned}\phi_t &= k\frac{\partial\mathcal{F}}{\partial\phi} \\ e_t &= -\nabla\left(m\nabla\left(\frac{\partial\mathcal{F}}{\partial e}\right)\right).\end{aligned}$$

Penrose and Fife showed global existence and uniqueness of a solution to the above model and also looked at the asymptotic behavior of the solution as $t \to \infty$. Horn [69], Sprekels and Zheng [92] and Horn, Laurençot and Sprekels [70] also explored the Penrose-Fife model.

With the appropriate choice of functions and constraints, it can be shown that the Penrose-Fife model is a generalization of the Phase Field model [56]. Kenmochi and Niezgódka [73], using the functional

$$\mathcal{F}[\phi,\theta] = \int_\Omega \}\tau(\theta) + \theta g(\phi) + \lambda(\phi) + \frac{k\theta}{2}|\nabla\phi|^2\}dx$$

in the Penrose-Fife model, derived an alternative phase transition model with the following dynamical equations

$$\begin{aligned}\rho_t &= \lambda_t(\phi) - \Delta u = f(t,x) \\ \phi_t + k\Delta\phi + g(\phi) &= \lambda'(\phi)u \\ \rho(u) &= \tau(\theta) + \theta\tau'(\theta)\end{aligned}$$

for which they also give results on global existence, uniqueness and asymptotic behavior of the solution as $t \to \infty$.

Chapter 2

A One Dimensional Model of Phase Transition

2.1 Introduction

We now examine a model of phase transition that uses an order parameter and includes temperature effects. Our model is similar to that of Gurtin and Fried [61] [63]. We present the dynamic equations following the derivation for the 1-D case as presented by Brandon and Rogers [10]. While Brandon and Rogers consider the temperature to be constant, we allow the temperature to vary. We consider a bar of length L with uniform cross section which undergoes contraction and expansion longitudinally. Our model will attempt to describe the longitudinal motions and variations in temperature of the bar.

Let $x \in [0, L]$ represent the reference position of the center of a cross section of the bar and let $t \in [0, \infty)$ be time. We then define the following kinematic and thermal quantities which we assume to depend on x and t:

u	longitudinal displacement
$v := \partial u/\partial t$	longitudinal velocity
$w := \partial u/\partial x$	longitudinal strain
ϕ	order parameter
$h := \partial \phi/\partial t$	order parameter rate of change
$p := \partial \phi/\partial x$	order parameter gradient
θ	average absolute temperature of a cross section
$g := \partial \theta/\partial x$	temperature gradient.

We restrict $\theta > 0$.

The order parameter, ϕ, has been given several physical interpretations in the literature. It may be construed as a measure of concentration or density of a binary fluid

[37]. In many instances, the order parameter, ϕ, is construed as a characterization of the phase of a material. On a microscopic level, it may represent the "atomic shuffle" of lattice structures. On a macrolocal level, it may actually represent the particular phase of the material at any point (x,t) [14]. Or on a level somewhere in between, it may represent a longer length scale average of the displacement, u. Gurtin and Fried [63] use an order parameter to account for a multiplicity of phases and/or phase variants. They identify phase boundaries as thin transition zones where the strain and order parameter have large gradients.

We now define the following quantities in order to describe the dynamics of the above quantities:

ρ	mass density per unit volume of reference length
σ	resultant contact force (stress) across a cross-section
f	external body force per unit cross-section
π	internal micro-local body force per unit cross-section
ξ	micro-local stress across a cross-section
γ	external micro-local force per unit cross-section
q	heat flux across a cross-section
r	external heat supply
ϵ	internal energy
η	entropy
$\psi := \epsilon - \theta\eta$	free energy.

All the above quantities are functions of x and t except ρ which is a function of x only.

2.2 Balance laws

We first assume three global balance laws:

Balance law of linear momentum: In accordance to Newton's Second Law, the time rate of change of linear momentum is equal to the total internal and external forces. Thus for every $[a,b] \subseteq [0,L]$, we have

$$\frac{\partial}{\partial t}\left(\int_a^b \rho(x)v(x,t)dx\right) = \sigma(b,t) - \sigma(a,t) + \int_a^b f(x,t)dx. \tag{2.1}$$

Balance law of micro-local forces: Following Gurtin and Fried's example [61] [63], we assume the micro-local forces associated with the order parameter do no net work. The corresponding balance of micro-local forces is: for every $[a,b] \subseteq [0,L]$,

$$0 = \xi(b,t) - \xi(a,t) + \int_a^b \{\pi(x,t) + \gamma(x,t)\}\, dx. \tag{2.2}$$

Note that we have not included any "micro-local momentum" terms. This is in keeping with Gurtin and Fried, but other authors take a different approach, see [79] [80] for example.
Balance law of energy: The First Law of Thermodynamics asserts that the time rate of change of the total energy is equal to the rate at which work is done to the system by all internal and external forces in addition to the rate at which heat interactions affects the system. Thus the balance law of energy for our system is: for every $[a,b] \subseteq [0,L]$,

$$\begin{aligned}\frac{\partial}{\partial t}\left(\int_a^b \left\{\epsilon(x,t) + \frac{\rho(x)}{2}|v(x,t)|^2\right\} dx\right) &= -q(b,t) + q(a,t) + \int_a^b r(x,t)dx \\ +\sigma(b,t)v(b,t) - \sigma(a,t)v(a,t) &+ \xi(b,t)\phi_t(b,t) - \xi(a,t)\phi_t(a,t) \\ +\int_a^b \{f(x,t)v(x,t) &+ \gamma(x,t)\phi_t(x,t)\}dx.\end{aligned} \tag{2.3}$$

To obtain the local form of the balance law of linear momentum we first take a derivative with respect to b:

$$\frac{\partial}{\partial b}\left(\frac{\partial}{\partial t}\left(\int_a^b \rho(x)v(x,t)dx\right)\right) = \frac{\partial}{\partial b}\left(\sigma(b,t) - \sigma(a,t) + \int_a^b f(x,t)dx\right). \tag{2.4}$$

Assuming v and ρ are sufficiently smooth, we change the order of the time derivative and the space derivative to get

$$\frac{\partial}{\partial t}\left(\frac{\partial}{\partial b}\left(\int_a^b \rho(x)v(x,t)dx\right)\right) = \frac{\partial}{\partial b}\left(\sigma(b,t) - \sigma(a,t) + \int_a^b f(x,t)dx\right).$$

Upon applying the Fundamental Theorem of Calculus and substituting x for b, we have

$$\rho(x)\frac{\partial v}{\partial t}(x,t) = \frac{\partial \sigma}{\partial x}(x,t) + f(x,t).$$

Using the alternate notation $\frac{\partial v}{\partial t}(x,t) \cong v_t$ and $\frac{\partial \sigma}{\partial x}(x,t) \cong \sigma_x$, we can write the above local balance law of momentum as

$$\rho v_t = \sigma_x + f. \tag{2.5}$$

Similarly, we obtain the local balance law of micro-local forces

$$0 = \xi_x + \pi + \gamma \tag{2.6}$$

and the local balance law of energy

$$\epsilon_t + \frac{\rho}{2}(|v|^2)_t = -q_x + r + [\sigma v]_x + [\xi\phi_t]_x + fv + \gamma\phi_t. \tag{2.7}$$

Upon expanding (2.7), we have

$$\epsilon_t + \rho v v_t = -q_x + r + \sigma v_x + \sigma_x v + \xi\phi_{t,x} + \xi_x\phi_t + fv + \gamma\phi_t.$$

Using equations (2.5) and (2.6) to substitute for ρv_t and ξ_x respectively, we have

$$\epsilon_t = -q_x + r + \sigma v_x + \xi \phi_{t,x} - \pi \phi_t.$$

Finally, replacing ϕ_t by h, the local balance law of energy reduces to

$$\epsilon_t = -q_x + r + \sigma v_x - \pi h + \xi h_x. \tag{2.8}$$

Dissipation Inequality: The Second Law of Thermodynamics asserts that the rate at which heat enters the system is no more than the total change in entropy. The best mathematical form of this is a matter of debate, but a common form is the following inequality: for every $[a,b] \subseteq [0,L]$,

$$\int_a^b r(x,t)dx - q(b,t) + q(a,t) \leq \int_a^b \left(\theta(x,t)\frac{\partial}{\partial t}\eta(x,t) - \frac{q(x,t)\frac{\partial}{\partial x}\theta(x,t)}{\theta(x,t)} \right) dx. \tag{2.9}$$

Upon rewriting (2.9), we have,

$$\int_a^b \left(r(x,t) - \frac{\partial}{\partial x}q(x,t) - \theta(x,t)\frac{\partial}{\partial t}\eta(x,t) + \frac{q(x,t)\frac{\partial}{\partial x}\theta(x,t)}{\theta(x,t)} \right) dx \leq 0. \tag{2.10}$$

Since $[a,b] \subseteq [0,L]$ is arbitrary, we have

$$r - q_x - \theta\eta_t + \frac{q\theta_x}{\theta} \leq 0. \tag{2.11}$$

Upon using the definition of the free energy to substitute $\psi_t + (\theta\eta)_t$ for ϵ_t in the local balance law of energy, (2.8), we have

$$r = \psi_t + (\theta\eta)_t + q_x - \sigma v_x + \pi h - \xi h_x. \tag{2.12}$$

Using (2.12) in (2.11), we have

$$\psi_t + \theta_{t\eta} + \pi h + \frac{q\theta_x}{\theta}dx \leq \sigma v_x + \xi h_x. \tag{2.13}$$

Assuming enough smoothness on u and ϕ and substituting g for θ_x and ϕ_t for h in (2.13), we have the local dissipation inequality

$$\psi_t + \theta_t\eta + \phi_t\pi + \frac{qg}{\theta} \leq w_t\sigma + p_t\xi. \tag{2.14}$$

2.3 Constitutive laws

We now assume that the bar is homogeneous and that the constitutive functions depend on the list

$$\Gamma(x,t) = (w(x,t), \phi(x,t), p(x,t), h(x,t), \theta(x,t), g(x,t)). \tag{2.15}$$

We then assume the constitutive relations

$$\begin{array}{rcl} \psi(x,t) & = & \hat{\psi}(\Gamma(x,t)) \\ \sigma(x,t) & = & \hat{\sigma}(\Gamma(x,t)) \\ \pi(x,t) & = & \hat{\pi}(\Gamma(x,t)) \\ \xi(x,t) & = & \hat{\xi}(\Gamma(x,t)) \\ q(x,t) & = & \hat{q}(\Gamma(x,t)) \\ \eta(x,t) & = & \hat{\eta}(\Gamma(x,t)). \end{array} \tag{2.16}$$

We follow the procedure laid out by Coleman and Noll [44] for thermoviscoelastic materials, that is, the constitutive functions (2.16) must satisfy the entropy inequality (2.14) for all processes. For a detailed explanation of the Coleman-Noll entropy principle, see e.g. Antman [1, pp. 441-8].

A process for a body consists of the fields u, ϕ and θ that satisfy the balance laws (2.5), (2.6) and (2.7). One of the main assumptions of this technique is that we can vary these processes "arbitrarily" by varying the external body force, f, the external micro-local force, γ, and the external heat supply, r, in any way we want. Hence, mathematically, all sufficiently smooth processes satisfy the balance laws (2.5), (2.6) and (2.7). Thus the constitutive relations (2.16) must satisfy the entropy inequality (2.14) identically.

We expand the dissipation inequality, (2.14), to obtain

$$\hat{\psi}_w w_t + \hat{\psi}_\phi \phi_t + \hat{\psi}_p p_t + \hat{\psi}_h h_t + \hat{\psi}_\theta \theta_t + \hat{\psi}_g g_t + \theta_t \hat{\eta} + \phi_t \hat{\pi} + \frac{\hat{q} g}{\theta} - w_t \hat{\sigma} + p \hat{\xi} \leq 0$$

or

$$(\hat{\psi}_w - \hat{\sigma}) w_t + (\hat{\psi}_\phi + \hat{\pi}) \phi_t + (\hat{\psi}_p - \hat{\xi}) p_t + (\hat{\psi}_\theta + \hat{\eta}) \theta_t + \hat{\psi}_h h_t + \hat{\psi}_g g_t + \frac{\hat{q} g}{\theta} \leq 0. \tag{2.17}$$

For any given time, by varying the process, we can vary varying $g, w_t, \phi_t, p_t, h_t, \theta_t$ or g_t independently. For example, we can choose a process such that, at a given (x,t), all rates and g are zero except w_t. Equation (2.17) simplifies to

$$(\hat{\psi}_w - \hat{\sigma}) w_t \leq 0. \tag{2.18}$$

Since w_t can take on any prescribed value, we must have

$$\hat{\psi}_w - \hat{\sigma} = 0$$

or

$$\hat{\psi}_w = \hat{\sigma}. \tag{2.19}$$

Using a similar argument, we can show

$$\begin{aligned} \hat{\psi}_p &= \hat{\xi} && (2.20)\\ \hat{\psi}_\theta &= -\hat{\eta} && (2.21)\\ \hat{\psi}_h &= 0 \\ \hat{\psi}_g &= 0. \end{aligned}$$

This implies that $\hat{\psi}$ is independent of h and g, i.e.,

$$\psi(x,t) = \hat{\psi}(w(x,t), \phi(x,t), p(x,t), \theta(x,t). \tag{2.22}$$

We should note that the above procedure cannot be used for $\phi_t = h$ or g since both $\hat{\pi}$ and $\hat{q}$ are dependent upon h and g. The inequality (2.17) thus reduces to

$$(\hat{\psi}_\phi + \hat{\pi})\phi_t + \frac{\hat{q}g}{\theta} \leq 0. \tag{2.23}$$

To ensure that the inequality (2.23) holds identically, we set

$$\begin{aligned} \hat{\pi} &= -\hat{\psi}_\phi - \hat{\beta}(\Gamma(x,t))h - \hat{K}(\Gamma(x,t))g && (2.24)\\ \hat{q} &= -\hat{k}(\Gamma(x,t))g - \hat{B}(\Gamma(x,t))h && (2.25) \end{aligned}$$

where $\hat{\beta}(\Gamma) > 0$ and $\hat{k}(\Gamma) > 0$ and where $\hat{B}(\Gamma)$ and $\hat{K}(\Gamma)$ satisfy

$$\hat{\beta}(\Gamma)h^2 + \hat{k}(\Gamma)g^2 + \left[\hat{K}(\Gamma) + \frac{\hat{B}(\Gamma)}{\theta}\right] hg \geq 0.$$

We consider the local balance laws (2.5), (2.6) and (2.8) using the constitutive functions defined in (2.16). Using the definition of ψ, we substitute $\hat{\epsilon} = \hat{\psi} + \theta\hat{\eta}$ in the local balance law of energy (2.8) to get

$$\hat{\psi}_t + \hat{\eta}\theta_t + \theta\hat{\eta}_t = -\hat{q}_x + r + \hat{\sigma}v_x - \hat{\pi}h + \hat{\xi}h_x.$$

Expanding $\hat{\psi}_t$ in the above equation yields

$$\hat{\psi}_w w_t + \hat{\psi}_\phi\phi_t + \hat{\psi}_p p_t + \hat{\psi}_\theta\theta_t + \hat{\eta}\theta_t + \theta\hat{\eta}_t = -\hat{q}_x + r + \hat{\sigma}v_x - \hat{\pi}h + \hat{\xi}h_x.$$

by (2.22). We now use equations (2.19)-(2.21) and $\phi_t = h$ to get

$$\hat{\sigma}w_t + \hat{\psi}_\phi h + \hat{\xi}p_t + \theta\hat{\eta}_t = -\hat{q}_x + r + \hat{\sigma}v_x - \hat{\pi}h + \hat{\xi}h_x.$$

Again, assuming enough smoothness on u and ϕ,

$$\begin{aligned} v_x &= w_t \\ h_x &= p_t, \end{aligned}$$

and we have

$$\hat{\psi}_\phi h + \theta\hat{\eta}_t = -\hat{q}_x + r - \hat{\pi}h.$$

Finally, substituting for $\hat{\pi}$ and $\hat{q}$ from equations (2.24) and (2.25), we have

$$\theta\hat{\eta}_t = +(\hat{k}(\Gamma)g + \hat{B}(\Gamma)h)_x + r + \hat{\beta}(\Gamma)h^2 + \hat{K}(\Gamma)gh.$$

Choosing $\hat{B}(\Gamma) = \hat{K}(\Gamma) = 0$, the local balance law of energy becomes

$$\theta\hat{\eta}_t - \hat{\beta}(\Gamma)h^2 = (\hat{k}(\Gamma)g)_x + r. \tag{2.26}$$

The local balance law of linear momentum is

$$\rho v_t = \hat{\sigma}_x + f \tag{2.27}$$

and the local balance law of micro-local forces using equation (2.24) to substitute for $\hat{\pi}$ is

$$0 = \hat{\xi}_x + -\hat{\psi}_\phi - \hat{\beta}(\Gamma)h + \gamma. \tag{2.28}$$

In terms of u, ϕ and θ, the local balance laws (2.26) - (2.28) take on the form

$$\begin{aligned} \rho u_{tt} &= \hat{\sigma}_x + f & (2.29) \\ \hat{\beta}(\Gamma)h &= \hat{\xi}_x - \hat{\psi}_\phi + \gamma & (2.30) \\ \theta\hat{\eta}_t - \hat{\beta}(\Gamma)\phi_t^2 &= r + (\hat{k}(\Gamma)\theta_x)_x. & (2.31) \end{aligned}$$

2.4 Constitutive choices

We now consider a particular constitutive choice for ψ. Let

$$\hat{\mathcal{G}}(w,\theta) := -c_\theta \theta \ln\left(\frac{\theta}{\theta_0}\right) + G(w,\theta)$$

where G is a polynomial in both w and θ. We then define

$$\hat{\psi}(w,p,\phi,\theta) := \hat{\mathcal{G}}(w,\theta) + \frac{1}{2}\begin{bmatrix} w & p & \phi \end{bmatrix}\begin{bmatrix} c_w & c_{wp} & c_{w\phi} \\ c_{pw} & c_p & c_{p\phi} \\ c_{\phi w} & c_{\phi p} & c_\phi \end{bmatrix}\begin{bmatrix} w \\ p \\ \phi \end{bmatrix}. \tag{2.32}$$

Assuming the coefficient matrix is symmetric, we have

$$\hat{\psi} = \hat{\mathcal{G}}(w,\theta) + \frac{1}{2}c_w w^2 + c_{wp}wp + c_{w\phi}w\phi + \frac{1}{2}c_p p^2 + c_{p\phi}p\phi + \frac{1}{2}c_\phi \phi^2.$$

Having chosen $\hat{\psi}$ thus, we have

$$\begin{aligned}
\hat{\sigma} = \hat{\psi}_w &= G_w(w,\theta) + c_w w + c_{wp}p + c_{w\phi}\phi && (2.33)\\
\hat{\xi} = \hat{\psi}_p &= c_{wp}w + c_p p + c_{p\phi}\phi && (2.34)\\
\hat{\eta} = -\hat{\psi}_\theta &= c_\theta + c_\theta \ln\left(\frac{\theta}{\theta_0}\right) - G_\theta(w,\theta) && (2.35)\\
\hat{\psi}_\phi &= c_{w\phi}w + c_{p\phi}p + c_\phi \phi. && (2.36)
\end{aligned}$$

Substituting equations (2.33)-(2.36) into the local balance laws (2.29)-(2.31) we have

$$\begin{aligned}
\rho u_{tt} &= G_{u_x}(u_x,\theta)_x + c_w u_{xx} + c_{wp}\phi_{xx} + c_{w\phi}\phi_x + f\\
\hat{\beta}(\Gamma)\phi_t &= c_{wp}u_{xx} + c_p\phi_{xx} - c_{w\phi}u_x - c_\phi\phi + \gamma\\
c_\theta\theta_t - \theta G_\theta(w,\theta)_t - \hat{\beta}(\Gamma)\phi_t^2 &= r + (\hat{k}(\Gamma)\theta_x)_x.
\end{aligned}$$

Upon choosing $c_{wp} = 0$ and absorbing $\frac{1}{2}c_w w^2$ into $G(w,\theta)$, the resulting differential equations are

$$\begin{aligned}
\rho u_{tt} &= G_{u_x}(u_x,\theta)_x + c_{w\phi}\phi_x + f && (2.37)\\
\hat{\beta}(\Gamma)\phi_t &= c_p\phi_{xx} - c_{w\phi}u_x - c_\phi\phi + \gamma && (2.38)\\
c_\theta\theta_t - \theta G_{\theta\theta}(w,\theta)\theta_t - \theta G_{\theta u_x}(u_x,\theta)u_{xt} - \hat{\beta}(\Gamma)\phi_t^2 &= r + (\hat{k}(\Gamma)\theta_x)_x. && (2.39)
\end{aligned}$$

We now continue with the constitutive choice for the potential energy function G. As in Brandon and Rogers [10], we choose a triple-well potential, symmetric about the central well. Whereas Brandon and Rogers chose a continuous piecewise quadratic, our potential takes the form of a eighth order polynomial in u_x while being linear in θ. We define $G : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ as follows:

$$\begin{aligned}
G(w,\theta) \;:=\; & \frac{w_1^2(3c - 36\theta - bw_1^2)}{144} + \frac{\theta w^2}{2} + \frac{bw^4}{24}\\
& - \frac{(3c + 18\theta + 2bw_1^2)w^6}{36w_1^4} + \frac{(3c + 12\theta - bw_1^2)w^8}{48w_1^6}
\end{aligned} \qquad (2.40)$$

Where b and c are constants, $\pm w_1$ are the equilibrium states in the outer wells and $w = 0$ is the equilibrium state in the inner well.

We note the following about the potential, G, as defined in (2.40):

- $G_{ww}(0,\theta) = \theta$.

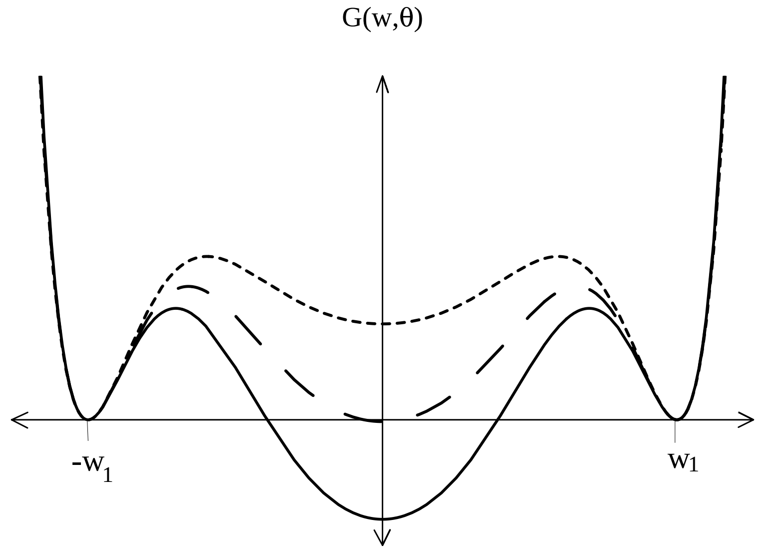

Figure 2.1: Triple-well potential G shown with various choices of θ.

- $G(\pm w_1, \theta) = 0$.
- $G_w(\pm w_1, \theta) = 0$.
- $G_w(0, \theta) = 0$.

This choice (2.40) of the potential function, G, simplifies the equation (2.39). That is, since $G_{\theta\theta}(w, \theta) = 0$, we have

$$c_\theta \theta_t - \theta G_{\theta u_x}(u_x, \theta) u_{xt} - \hat{\beta}(\Gamma)\phi_t^2 = r + (\hat{k}(\Gamma)\theta_x)_x. \tag{2.41}$$

2.5 Regularization of the model

In this section we present two systems of equations, one for the temperature independent case, the other for the temperature dependent case. In both cases, viscosity terms, parameterized by ϵ_1 and ϵ_2, have been added to the local balance law of momentum represented as a first order system. The viscosity terms regularize the system, that is, we now have a parabolic system of equations. As was seen in the discussion of Gibbs' double-well model in Chapter 1, the existence of multiple solutions is quite probable for the unregularized system. We shall show in Chapter 3 that for the temperature independent problem, the parabolic system has a unique solution dependent upon our choice of ϵ_1 and ϵ_2. For small values of ϵ_1 and ϵ_2 the parabolic system may be a good model representative of solid-solid phase transitions.

2.5.1 The temperature independent system

First we look at the temperature independent case. We consider temperature to be constant, that is, $\theta = \theta_0$ and ignore the heat equation (2.39). Then the system of equations (2.37),(2.38) and (2.41) reduce to

$$\rho u_{tt} = G_{u_x}(u_x, \theta_0)_x + c_{w\phi}\phi_x + f \tag{2.42}$$
$$\hat{\beta}(\Gamma)\phi_t = c_p\phi_{xx} - c_{w\phi}u_x - c_\phi\phi + \gamma \tag{2.43}$$

We now convert equations (2.42) and (2.43) to a first order system in time and add viscosity and 'mass viscosity' to regularize the problem. We also set f and γ to zero. The system of regularized equations is

$$w_t(t,x) = v_x(t,x) + \epsilon_1^2 w_{xx}(t,x) \tag{2.44}$$
$$\rho v_t(t,x) = G'(w(t,x))_x - \gamma\phi_x(t,x) + \epsilon_2^2 v_{xx}(t,x) \tag{2.45}$$
$$\hat{\beta}(\Gamma)\phi_t(t,x) = \gamma w(t,x) - \alpha\phi(t,x) + \epsilon_3^2\phi_{xx}(t,x) \tag{2.46}$$

here $\epsilon_1 > 0$ and $\epsilon_2 > 0$. We choose the following initial conditions

$$w(t_0,x) = w_0(x) \tag{2.47}$$
$$v(t_0,x) = v_0(x) \tag{2.48}$$
$$\phi(t_0,x) = \phi_0(x) \tag{2.49}$$

and boundary conditions

$$w_x(t,0) = 0 \qquad w_x(t,L) = 0 \tag{2.50}$$
$$v(t,0) = 0 \qquad v(t,L) = g(t) \tag{2.51}$$
$$\phi_x(t,0) = 0 \qquad \phi_x(t,L) = 0 \tag{2.52}$$

where $g \in C^2(0,\infty)$ is a forcing function, w_0, v_0 and ϕ_0 are continuous functions from $[0,1]$ to the real numbers. The term $\epsilon_2^2 v_{xx}(t,x)$ represents Newtonian viscosity, while the mass viscosity term, $\epsilon_1^2 w_{xx}(t,x)$, is purely mathematical, chosen to ensure the system is parabolic.

2.5.2 The temperature dependent system

We now turn our attention to the temperature dependent case. We now convert equations (2.42)-(2.41) to a first order system in time and, again, add viscosity and 'mass viscosity' to regularize the problem. We set f, γ and r equal to zero. We also set $v_x = u_{xt}$. The system of regularized equations is

$$\begin{aligned} w_t &= v_x + \epsilon_1^2 w_{xx} && (2.53) \\ \rho v_t &= G_w(w,\theta)_x - \gamma\phi_x + \epsilon_2^2 v_{xx} && (2.54) \\ \beta(\Gamma)\phi_t &= \gamma w - \alpha\phi + \epsilon_3^2 \phi_{xx} && (2.55) \\ c_\theta \theta_t - \hat{\beta}(\Gamma)\phi_t^2 &= (\hat{k}(\Gamma)\theta_x)_x + \theta G_{\theta w}(w,\theta) v_x. && (2.56) \end{aligned}$$

We choose the following initial conditions

$$\begin{aligned} w(t_0,x) &= w_0(x) && (2.57) \\ v(t_0,x) &= v_0(x) && (2.58) \\ \phi(t_0,x) &= \phi_0(x). && (2.59) \\ \theta(t_0,x) &= \theta_0(x) && (2.60) \end{aligned}$$

and boundary conditions

$$\begin{aligned} w_x(t,0) = 0 &\qquad w_x(t,L) = 0 && (2.61) \\ v(t,0) = 0 &\qquad v(t,L) = g(t) && (2.62) \\ \phi_x(t,0) = 0 &\qquad \phi_x(t,L) = 0 && (2.63) \\ \theta(t,0) = \alpha_\theta &\qquad \theta(t,L) = \beta_\theta && (2.64) \end{aligned}$$

where α_θ and β_θ are constants, $g \in C^2(0,\infty)$ is a forcing function, w_0, v_0, ϕ_0 and θ_0 are continuous functions from $[0,1]$ to the real numbers.

Chapter 3

Existence of a Solution of the Regularized, Temperature Independent Model

3.1 Introduction

The goal of this chapter is to prove the existence of a unique classical solution of the initial value boundary problem (2.44)-(2.49) with homogeneous boundary conditions. We begin by stating the main theorem.

Theorem 3.1 *Suppose w_0, v_0 and $\phi_0 \in H_0^1(0,l)$. Then there is a real number, $t_1 > 0$, such that there exists unique solutions, $\bar{w}, \bar{v}$ and $\bar{\phi}$, of the initial value boundary problem (2.44)-(2.49) with*

$$\begin{aligned}
\bar{w} &\in C([0,t_1); H_0^1(0,l)) \cap C^1((0,t_1); H_0^1(0,l)) \cap C((0,t_1); H^2(0,l)) \\
\bar{v} &\in C([0,t_1); H_0^1(0,l)) \cap C^1((0,t_1); H_0^1(0,l)) \cap C((0,t_1); H^2(0,l)) \\
\bar{\phi} &\in C([0,t_1); H_0^1(0,l)) \cap C^1((0,t_1); H_0^1(0,l)) \cap C((0,t_1); H^2(0,l)).
\end{aligned}$$

3.2 Definitions

We proceed with preliminary definitions and theory needed to establish the existence and uniqueness of a solution to our problem. The following definitions are standard mathematical terminology and may be found in sources such as Zeidler for operator theory [96], Pazy for semigroup theory [84] and Henry for initial value problems [68].

3.2.1 Operator theory

Let X be a Hilbert space with norm $\|\cdot\|_X$ and inner product $\langle\cdot,\cdot\rangle_X$. Let $\mathbf{A}$ be a linear operator from X to X with dense domain $\mathcal{D}(\mathbf{A})$. We say $\mathbf{A}$ is *symmetric* if

$$\langle \mathbf{A}u, v\rangle_X = \langle u, \mathbf{A}v\rangle_X$$

for all u, v in $D(\mathbf{A})$. The *adjoint* of $\mathbf{A}$, $\mathbf{A}^*$, is defined as follows. We say $v \in D(\mathbf{A}^*) \subset X$ if and only if there exists $v^* \in X$ such that

$$\langle \mathbf{A}u, v\rangle_X = \langle u, v^*\rangle_X$$

for all u in $D(\mathbf{A})$. For each $v \in D(\mathbf{A}^*)$, the adjoint is defined by $v^* = \mathbf{A}^*v$. $\mathbf{A}$ is called *self-adjoint* if $\mathbf{A} = \mathbf{A}^*$. We say $\mathbf{A}$ is *semibounded* if there exists a real constant c such that

$$\langle \mathbf{A}u, u\rangle_X \quad \geq \quad c\|u\|_X^2$$

for all u in $D(\mathbf{A})$ and *strongly monotone* if $c > 0$. Suppose $\mathbf{A}$ is symmetric and strongly monotone, the *energetic space* of $\mathbf{A}$, X_E, is the completion of $D(\mathbf{A})$ with respect to the norm induced by the inner product $\langle\cdot,\cdot\rangle_E$ where

$$\langle u, v\rangle_E = \langle \mathbf{A}u, v\rangle_X$$

for all u, v in $D(\mathbf{A})$.

In order to proceed, we consider the initial value problem (2.44)-(2.49) as an abstract problem. The following theorem enables us to do so.

Theorem 3.2 (Friedrich) *Suppose $\mathbf{A} : D(\mathbf{A}) \subset X \to X$ is linear, densely defined, symmetric and strongly monotone with constant $c > 0$. Then we have the following.*

1. *There exists a self-adjoint extension $\mathbf{A}_F : D(\mathbf{A}_F) \subseteq X \to X$ of $\mathbf{A}$ with $D(\mathbf{A}_F) \subseteq X_E \subseteq X$ and $\langle \mathbf{A}_F u, u\rangle_X \geq c\|u\|_X^2$ for all $u \in D(\mathbf{A}_F)$.*

2. *The inverse operator $\mathbf{A}_F^{-1} : X \to X$ exists and is linear, continuous and self-adjoint. Thus, for each $f \in X$, the equation $\mathbf{A}_F u = f$ has a unique solution, $\bar{u} \in D(\mathbf{A}_F)$.*

3. *$\mathbf{A}_F^{-1} : X \to X_E$ is linear and continuous, here X_E^* is the dual space of X_E.*

4. *The embeddings $X_E \subseteq X \subseteq X_E^*$ are continuous.*

5. *$\mathbf{A}_F$ has the extension $\mathbf{A}_E : X_E \to X_E^*$ where $\mathbf{A}_E$ is a linear homeomorphism with $\langle \mathbf{A}_E u, u\rangle_X = \|u\|_E^2$ for all $u \in X_E$. Moreover, $\mathbf{A}_F^{-1} f = \mathbf{A}_E^{-1} f$ for all $f \in X$.*

6. *If the embedding $X_E \subseteq X$ is compact, then $\mathbf{A}_F^{-1} : X \to X$ is compact.*

The proof of Theorem 3.2 can be found in Zeidler [96, pp. 129-31]. The following corollary provides us with a complete orthonormal set of eigenvectors for $\mathbf{A}_F$.

Corollary 3.3 *Suppose* $\mathbf{A} : D(\mathbf{A}) \subset X \to X$ *is linear, densely defined, symmetric and strongly monotone with constant* $c > 0$*. Suppose, further, that* $\dim X = \infty$ *and the embedding* $X_E \subset X$ *is compact. Then,*

1. $\mathbf{A}_F : D(\mathbf{A}_F) \subseteq X \to X$ *has a countable system of eigensolutions* $\{u_n, \lambda_n\}$ *which contains all the eigenvalues of* $\mathbf{A}_F$*.*

2. *All the eigenvalues of* $\mathbf{A}_F$ *have finite multiplicity. Furthermore,* $\lambda_n \geq c$ *for all* n *and* $\lambda_n \to \infty$ *as* $n \to \infty$*.*

3. *The eigenvectors* $\{u_n\}$ *form a complete orthonormal system in* X*.*

The proof of Corollary 3.3 can be found in Zeidler [96, p. 127]. Using Corollary 3.3 and the following lemma we are able to represent $\mathbf{A}u$ in series notation using the eigenpairs of $\mathbf{A}$.

Lemma 3.4 *Let* $\mathbf{A} : D(\mathbf{A}) \subset X \to X$ *be self-adjoint on a separable Hilbert space* X*. Suppose* $\mathbf{A}$ *possesses a complete orthonormal system of eigenvectors* $\{u_n\}$ *in* X*. Then*

$$\mathbf{A}u = \sum_n \lambda_n \langle u_n, u \rangle_X u_n$$

for all u *in* $D(\mathbf{A})$*.*

Proof. For all $v \in X$,

$$v = \sum_n \langle v, u_n \rangle_X u_n,$$

since $\{u_n\}$ is complete. If $u \in D(\mathbf{A})$, then

$$\langle \mathbf{A}u, u_n \rangle_X = \langle u, \mathbf{A}u_n \rangle_X = \lambda_n \langle u, u_n \rangle_X.$$

Thus

$$\mathbf{A}u = \sum_n \langle \mathbf{A}u, u_n \rangle_X u_n = \sum_n \lambda_n \langle u, u_n \rangle_X u_n.$$

■

For each function, $\tilde{f} : \mathbb{R} \to \mathbb{R}$, we define $\tilde{f}(\mathbf{A})$ as follows:

$$\tilde{f}(\mathbf{A})u = \sum_n \tilde{f}(\lambda_n) \langle u_n, u \rangle_X u_n \tag{3.1}$$

for all $u \in D(\tilde{f}(\mathbf{A}))$ where

$$D(\tilde{f}(\mathbf{A})) = \{u \in X : \sum_n |\tilde{f}(\lambda_n)|^2 |\langle u_n, u\rangle_X|^2 < \infty\}.$$

The operator $f(\mathbf{A})$ is self-adjoint for self-adjoint operators with a complete orthonormal system of eigenvectors:

Lemma 3.5 *Let $\mathbf{A} : D(\mathbf{A}) \subset X \to X$ be self-adjoint on a separable Hilbert space X. Suppose $\mathbf{A}$ possesses a complete orthonormal system of eigenvectors $\{u_n\}$ in X. Then the operator $\tilde{f}(\mathbf{A})$, as defined by (3.1), is self-adjoint for each function $\tilde{f} : \mathbb{R} \to \mathbb{R}$.*

Proof. Let $\mathbf{B} = f(\mathbf{A})$ and let $\mathbf{B}^*$ denote the adjoint operator. B is symmetric, i.e., $\mathbf{B} \subseteq \mathbf{B}^*$, since for all $u, v \in D(\mathbf{B})$,

$$\langle \mathbf{B}u, v\rangle_X = \sum_n f(\lambda_n)\langle u, u_n\rangle_X \langle v, u_n\rangle_X = \langle u, \mathbf{B}v\rangle_X.$$

To show $\mathbf{B}^* \subseteq \mathbf{B}$, let $u \in D(\mathbf{B}^*)$. Since

$$\langle \mathbf{B}^* u, u_n\rangle_X = \langle u, \mathbf{B}u_n\rangle_X = f(\lambda_n)\langle u, u_n\rangle_X,$$

we have

$$\mathbf{B}^* u = \sum_n \langle \mathbf{B}^* u, u_n\rangle_X u_n = \sum_n f(\lambda_n)\langle u, u_n\rangle_X u_n.$$

Hence, $u \in D(\mathbf{B})$ and $\mathbf{B}$ is self-adjoint. ■

Suppose $\mathbf{A} : X \to X$ is self-adjoint and strongly monotone with bound $c > 0$ on a separable Hilbert space with $\dim X = \infty$. We define the operator $\mathbf{A}^\alpha : X \to X$ for $\alpha > 0$ as follows:

$$\mathbf{A}^\alpha u = \sum_n \lambda_n^\alpha \langle u_n, u\rangle_X u_n$$

for all u in $X^\alpha = D(\mathbf{A}^\alpha)$ where

$$D(\mathbf{A}^\alpha) := \{u \in X : \sum_n |\lambda_n^\alpha|^2 |\langle u_n, u\rangle_X|^2 < \infty\}.$$

By Lemma 3.5, $\mathbf{A}^\alpha$ is self-adjoint. $\mathbf{A}^\alpha$ is strongly monotone since

$$\begin{aligned}
\langle \mathbf{A}^\alpha u, u\rangle_X &= \langle \sum_n \lambda_n^\alpha \langle u_n, u\rangle_X u_n, u\rangle_X \\
&= \langle \sum_n \lambda_n^\alpha \langle u_n, u\rangle_X u_n, \sum_n \lambda_n \langle u_n, u\rangle_X u_n\rangle_X \\
&= \langle \sum_n \lambda_n^{\alpha-1} \lambda_n \langle u_n, u\rangle_X u_n, \sum_n \lambda_n \langle u_n, u\rangle_X u_n\rangle_X \\
&\geq c^{(\alpha-1)} \langle \sum_n \lambda_n \langle u_n, u\rangle_X u_n, \sum_n \lambda_n \langle u_n, u\rangle_X u_n\rangle_X \\
&= c^{(\alpha-1)} \langle u, u\rangle_X = c^{(\alpha-1)} \|u\|_X^2
\end{aligned}$$

where we have used $(\lambda_n)^{(\alpha-1)} > c^{(\alpha-1)} > 0$.

We define two norms on X^α. The first is the *graph norm* on X^α, defined by

$$\|u\|_\alpha^\star := \|u\|_X + \|\mathbf{A}^\alpha u\|_X.$$

The second is defined by

$$\|u\|_\alpha := \|\mathbf{A}^\alpha u\|_X.$$

We now show that $\|u\|_\alpha^\star$ and $\|u\|_\alpha$ are indeed norms on X^α. Moreover, these two norms are equivalent on X^α.

Lemma 3.6 $\|u\|_\alpha^\star$ *is a norm on* X^α.

Proof. Let $u, v \in X^\alpha$ and $a \in \mathbb{R}$.

1. Since $\|\cdot\|_X$ is a norm, we have

$$\|u\|_\alpha^\star = \|u\|_X + \|\mathbf{A}^\alpha u\|_X \geq 0.$$

Let $u = 0$, then $\|u\|_\alpha^\star = 0$. Now suppose $\|u\|_\alpha^\star = 0$. By definition,

$$0 = \|u\|_X + \|\mathbf{A}^\alpha u\|_X \geq 0$$

which in turn implies $u = 0$.

2. By the linearity of $\mathbf{A}^\alpha$ and the properties of the norm $\|\cdot\|_X$, we have

$$\begin{aligned} \|au\|_\alpha^\star &= \|au\|_X + \|\mathbf{A}^\alpha(au)\|_X \\ &= |a|\|u\|_X + |a|\|\mathbf{A}^\alpha u\|_X \\ &= |a|\|u\|_\alpha^\star \end{aligned}$$

3. Again, by the linearity of $\mathbf{A}^\alpha$ and the properties of the norm $\|\cdot\|_X$, we have

$$\begin{aligned} \|u+v\|_\alpha^\star &= \|u+v\|_X + \|\mathbf{A}^\alpha(u+v)\|_X \\ &= \|u+v\|_X + \|\mathbf{A}^\alpha u + \mathbf{A}^\alpha v)\|_X \\ &\leq \|u\|_X + \|v\|_X + \|\mathbf{A}^\alpha u\|_X + \|\mathbf{A}^\alpha v)\|_X \\ &= \|u\|_\alpha^\star + \|v\|_\alpha^\star \end{aligned}$$

■

Lemma 3.7 $\|u\|_\alpha$ *is a norm on* X^α.

Proof. Let $u, v \in X^\alpha$ and $a \in \mathbb{R}$.

1. Since $\|\cdot\|_X$ is a norm, we have
$$\|u\|_\alpha = \|\mathbf{A}^\alpha u\|_X \geq 0.$$
Let $u = 0$, then $\|u\|_\alpha = 0$. Now suppose $\|u\|_\alpha = 0$. Since $\|\mathbf{A}^\alpha u\|_X = 0$ and $\{u_n\}$ is an orthonormal system,
$$0 = \|\mathbf{A}^\alpha u\|_X^2 = \langle \mathbf{A}^\alpha u, \mathbf{A}^\alpha u\rangle_X = \sum_n |\lambda_n^\alpha|^2 |\langle u_n, u\rangle_X|^2.$$
This implies
$$0 = |\lambda_j^\alpha|^2 |\langle u_j, u\rangle_X|^2$$
for all $j = 1, 2, 3, \cdots$. By Corollary 3.3, the eigenvalues of $\mathbf{A}^\alpha$ satisfy $\lambda_j^\alpha > 0$, for all $j = 1, 2, 3, \cdots$, thus
$$0 = \langle u_j, u\rangle_X$$
for all $j = 1, 2, 3, \cdots$ which in turn implies $u = 0$ since $\{u_n\}$ is complete.

2. By the linearity of $\mathbf{A}^\alpha$ and the properties of the norm $\|\cdot\|_X$, we have
$$\begin{aligned} \|au\|_\alpha &= \|\mathbf{A}^\alpha (au)\|_X \\ &= |a|\|\mathbf{A}^\alpha u\|_X \\ &= |a|\|u\|_\alpha \end{aligned}$$

3. Similarly, by the linearity of $\mathbf{A}^\alpha$ and the properties of the norm $\|\cdot\|_X$, we have
$$\begin{aligned} \|u+v\|_\alpha &= \|\mathbf{A}^\alpha (u+v)\|_X \\ &= \|\mathbf{A}^\alpha u + \mathbf{A}^\alpha v\|_X \\ &\leq \|\mathbf{A}^\alpha u\|_X + \|\mathbf{A}^\alpha v\|_X \\ &= \|u\|_\alpha + \|v\|_\alpha \end{aligned}$$

■

To show the equivalence of the two norms, we need to establish the inequality
$$\|\mathbf{A}^\alpha u\|_X \geq d\|u\|_X \tag{3.2}$$
for all $u \in X^\alpha$ and for some $d > 0$. Let $u \in X^\alpha$,
$$\begin{aligned} \|\mathbf{A}^\alpha u\|_X^2 = \langle \mathbf{A}^\alpha u, \mathbf{A}^\alpha u\rangle_X &= \langle \sum_n \lambda_n^\alpha \langle u_n, u\rangle_X u_n, \sum_n \lambda_n^\alpha \langle u_n, u\rangle_X u_n\rangle_X \\ &= \langle \sum_n \lambda_n^{\alpha-1}\lambda_n \langle u_n, u\rangle_X u_n, \sum_n \lambda_n^{\alpha-1}\lambda_n \langle u_n, u\rangle_X u_n\rangle_X \\ &\geq c^{(\alpha-1)^2} \langle \sum_n \lambda_n \langle u_n, u\rangle_X u_n, \sum_n \lambda_n \langle u_n, u\rangle_X u_n\rangle_X \\ &= d^2 \langle u, u\rangle_X = d^2 \|u\|_X^2 \end{aligned}$$

where, again, we have used $\lambda_n^{(\alpha-1)} > d = c^{(\alpha-1)} > 0$. Having established (3.2), we have

$$(d+1)\|\mathbf{A}^\alpha u\|_X \geq d(\|u\|_X + \|\mathbf{A}^\alpha u\|_X) \geq d\|\mathbf{A}^\alpha u\|_X$$

or, equivalently,

$$\frac{d+1}{d}\|u\|_\alpha \geq \|u\|_\alpha^\star \geq \|u\|_\alpha.$$

Thus the norm $\|\cdot\|_\alpha$ is an equivalent norm to $\|\cdot\|_\alpha^*$ on X^α.

Example 3.8 Let Ω be a bounded subset of $\mathbb{R}^n$ (all applications in this thesis are for $n = 1$). The space $C_0^\infty(\Omega)$ is the space of all infinitely differentiable functions on Ω with compact support, that is, $u(x) = 0$ for $x \in \partial\Omega$. The norm on $C_0^\infty(\Omega)$ is defined by

$$\|u\|_{C_0^\infty(\Omega)} = \max_{x\in\Omega} |u(x)|.$$

The space $L^2(\Omega)$ is the space of square integrable functions with norm

$$\|u\|_{L^2(\Omega)} = \{\int_\Omega |u(x)|^2 dx\}^{\frac{1}{2}}.$$

We define the L^2 inner product by

$$\langle u, v\rangle_{L^2(\Omega)} = \int_\Omega u(x)v(x)dx$$

for $u, v \in L^2(\Omega)$. The Hilbert space $H^m(\Omega)$ is the space of all functions that are in $L^2(\Omega)$ and that have derivatives up to order m in $L^2(\Omega)$. For example a function u is in $H^2(\Omega)$ if $u, \dfrac{\partial u}{\partial x_i}$ and $\dfrac{\partial^2 u}{\partial x_i \partial x_j}$ are all in $L^2(\Omega)$ for $1 \leq i, j \leq n$. The norm on $H^2(\Omega)$ is defined by

$$\|u\|_{H^2(\Omega)} = \{\|u\|_{L^2(\Omega)} + \sum_{i=1}^n \|\frac{\partial u}{\partial x_i}\|_{L^2(\Omega)} + \sum_{i,j=1}^n \|\frac{\partial^2 u}{\partial x_i \partial x_j}\|_{L^2(\Omega)}\}^{\frac{1}{2}}.$$

The space $H_0^m(\Omega)$ is the space of functions in $H^m(\Omega)$ with compact support.

Consider the differential operator $-\mathbf{\Delta} : C_0^\infty(\Omega) \subset L^2(\Omega) \to L^2(\Omega)$. We note that $-\mathbf{\Delta}$ is linear and symmetric with respect to the L^2 inner product and densely defined in $X = L^2(\Omega)$. Using Poincare's inequality, there exists $\hat{c} > 0$ such that

$$\langle -\mathbf{\Delta} u, u\rangle_{L^2(\Omega)} = \langle u_x, u_x\rangle_{L^2(\Omega)} \geq \hat{c}\langle u, u\rangle_{L^2(\Omega)} = \hat{c}\|u\|_{L^2(\Omega)}^2$$

for all u in $C_0^\infty(\Omega)$. Thus $-\mathbf{\Delta}$ is strongly monotone. The energetic space, X_E, is the completion of $C_0^\infty(\Omega)$ with respect to the inner product

$$\langle -\mathbf{\Delta} u, v\rangle_{L^2(\Omega)} = \langle u_x, v_x\rangle_{L^2(\Omega)}$$

for all $u, v \in C_0^\infty(\Omega)$. Poincare's inequality ensures that this is equivalent to the $H^1(\Omega)$ norm on $C_0^\infty(\Omega)$. Since $H_0^1(\Omega)$ is defined to be the completion of $C_0^\infty(\Omega)$ in the $H^1(\Omega)$ norm, we have $X_E = H_0^1(\Omega)$ and $X_E^* = H^{-1}(\Omega)$.

Friedrich's Theorem ensures the existence of the operator $-\mathbf{\Delta}_F : D(-\mathbf{\Delta}_F) \subseteq H_0^1(\Omega) \to L^2(\Omega)$ which is linear, self-adjoint and strongly monotone. Moreover, $-\mathbf{\Delta}_F$ has the extension $-\mathbf{\Delta}_E : H_0^1(\Omega) \to H^{-1}(\Omega)$ such that

$$\langle -\mathbf{\Delta}_E u, u \rangle = \|u\|_E^2$$

for all $u \in H_0^1(\Omega)$. It can be shown, [96, p. 184], that $D((-\mathbf{\Delta}_F)^{\frac{1}{2}}) = D(-\mathbf{\Delta}_E)$ and accordingly

$$X^{\frac{1}{2}} = H_0^1(\Omega). \tag{3.3}$$

To see the relationship between the abstract results of the Friedrich Theorem and more specific results for elliptic differential equations we consider the bilinear form $B : H_0^1(\Omega) \times H_0^1(\Omega) \to \mathbb{R}$ where $B(u, v) = \langle -\mathbf{\Delta}_E u, v \rangle$ for $(u, v) \in D(B)$. Using Hölder's inequality,

$$\begin{aligned} |B(u,v)| &= |\langle -\mathbf{\Delta}_E u, v \rangle_{L^2(\Omega)}| \\ &= |\langle \nabla u, \nabla v \rangle_{L^2(\Omega)}| \\ &\leq \int_\Omega |\nabla u \nabla v| dx \\ &\leq \|u\|_{H^1(\Omega)} \|v\|_{H^1(\Omega)} \end{aligned} \tag{3.4}$$

for all $(u, v) \in D(B)$. Since (3.4) holds and $-\mathbf{\Delta}_E$ is strictly monotone we can apply the Lax-Milgram Lemma to guarantee that for every $f \in H^{-1}(\Omega)$ there exists a unique $u \in H_0^1(\Omega)$ such that $B(u, v) = f(u)$ for all $v \in H_0^1(\Omega)$.

Thus, the solution generated by the Lax-Milgram Lemma is the solution of the energetic extension, $-\mathbf{\Delta}_E$, of the Laplacian, $-\mathbf{\Delta}$. The Friedrich extension, $-\mathbf{\Delta}_F$, is identified by the following elliptic regularity result for the Laplacian, specifically, it identifies $D(-\mathbf{\Delta}_F)$.

Theorem 3.9 *(Elliptic Regularity) Given the differential operator $-\mathbf{\Delta}$ of the form*

$$-\mathbf{\Delta} u := -\sum_{i=1}^{n} \frac{\partial^2 u}{\partial x_i^2}$$

with corresponding bilinear form

$$B(u, v) := \int_\Omega \nabla u \cdot \nabla v dx.$$

Suppose $f \in L^2(\Omega)$ and $\partial\Omega$ is of class C^2. Let $u \in H_0^1(\Omega)$ be a weak solution of the Dirichlet problem for $-\mathbf{\Delta} u = f$. Then $u \in H^2(\Omega)$ and

$$\|u\|_{H^2(\Omega)} \leq c(\|u\|_{L^2(\Omega)} + \|f\|_{L^2(\Omega)}).$$

The proof of a more general elliptic regularity theorem may be found in Renardy and Rogers [87, pp. 323-34]. The Friedrich Theorem guarantees the existence of a unique solution, $\tilde{u}$, to the Dirichlet problem for $-\mathbf{\Delta}_F u = f$ for each $f \in L^2(\Omega)$. From the same theorem we know, given $f \in L^2(\Omega)$,

$$\tilde{u} = -\mathbf{\Delta}_F^{-1} f = -\mathbf{\Delta}_E^{-1} f \in H_0^1(\Omega).$$

Thus by Elliptic Regularity, we have $\tilde{u} \in H^2(\Omega)$. Therefore $D(-\mathbf{\Delta}_F) = H^2(\Omega) \cap H_0^1(\Omega)$.

3.2.2 Semigroups

A *semigroup*, $\{S(t)\}$, on X consists of a family of bounded linear operators $S(t) : X \to X$ for all $t \in \mathbb{R}_+ = [0, \infty)$ satisfying

$$\begin{aligned} S(t+s) &= S(t)S(s) \;\; \forall\, t, s \in \mathbb{R}_+ \\ S(0) &= I \end{aligned}$$

where I is the identity operator. Let $D(\mathbf{A})$ be the set of u in X for which

$$\lim_{t \to 0^+} \frac{S(t)u - u}{t}$$

exists. We define the linear operator $\mathbf{A}$ by

$$\mathbf{A}u = \lim_{t \to 0^+} \frac{S(t)u - u}{t}$$

for all u in $D(\mathbf{A})$. The operator $\mathbf{A} : \mathcal{D}(\mathbf{A}) \subseteq X \to X$ is called the *generator* of the semigroup $\{S(t)\}$. The semigroup $\{S(t)\}$ is said to be *strongly continuous* if and only if $t \mapsto S(t)u$ is continuous on $\mathbb{R}_+$ for all u in X, that is,

$$\lim_{t \to s} \|S(t)u - S(s)u\|_X = 0$$

for all $u \in D(\mathbf{A})$. A strongly continuous semigroup of bounded linear operators on X is called a C_0 semigroup.

We continue with some general results concerning C_0 semigroups.

Theorem 3.10 *If $\mathbf{A} : D(\mathbf{A}) \subseteq X \to X$ is a densely defined linear self-adjoint strongly monotone operator on $D(\mathbf{A})$, then $-\mathbf{A}$ is the generator of a linear strongly continuous semigroup, $\{S(t)\}$. We write $\{S(t)\} = \{e^{-t\mathbf{A}}\}$.*

The proof of a more generalized version of Theorem 3.10 can be found in Zeidler [96, pp. 162-4].

Theorem 3.11 *Let $\mathbf{A}$ be the infinitesimal generator of a C_0 semigroup, $\{S(t)\}$. Then for $x \in D(\mathbf{A})$ and $t > 0$, we have $S(t)x \in D(\mathbf{A})$ and*

$$\frac{d}{dt}S(t)x = \mathbf{A}S(t)x.$$

Proof. Let $x \in D(\mathbf{A})$ and $h > 0$. Then

$$\frac{S(h) - I}{h}S(t)x = S(t)\left(\frac{S(h) - I}{h}\right)x \to S(t)\mathbf{A}x \tag{3.5}$$

as $h \to 0^+$. Thus, $S(t)x \in D(\mathbf{A})$ and $\mathbf{A}S(t)x = S(t)\mathbf{A}x$.

Now, (3.5) implies that

$$\frac{d^+}{dt}S(t)x = \mathbf{A}S(t)x = S(t)\mathbf{A}x,$$

i.e., the right derivative exists. We now show that the left derivative exists for $t > 0$ and equals $S(t)\mathbf{A}x$. We note that

$$\begin{aligned} \lim_{h \to 0^+}\left[\frac{S(t)x - S(t-h)x}{h} - S(t)\mathbf{A}x\right] &= \lim_{h \to 0^+} S(t-h)\left[\frac{S(h)x - x}{h} - \mathbf{A}x\right] \\ &\quad + \lim_{h \to 0^+}(S(t-h)\mathbf{A}x - S(t)\mathbf{A}x) = 0 \end{aligned}$$

since $x \in D(\mathbf{A})$, $\|S(t-h)\|$ is bounded on $0 \le h \le t$ and $S(t)$ is strongly continuous. ■

The following theorem gives us bounds on the operators $\mathbf{A}^\alpha e^{-t\mathbf{A}}$ and $(e^{-t\mathbf{A}} - \mathbf{I})$.

Theorem 3.12 *Let $\mathbf{A}$ be a self-adjoint, densely defined and monotone operator on a separable Hilbert space, X. Suppose $\mathbf{A}$ possesses a complete orthonormal system of eigenvectors $\{u_n\}$ in X. Then there exists a constant $C > 0$ depending on $\alpha \in (0, 1)$ such that the following are true:*

1. $\|(e^{-t\mathbf{A}} - \mathbf{I})u\| \le Ct^\alpha \|\mathbf{A}^\alpha u\|$ *for all* $u \in D(\mathbf{A}^\alpha)$ *and* $t > 0$.
2. $\|\mathbf{A}^\alpha e^{-t\mathbf{A}}\| \le Ct^{-\alpha}$ *and* $e^{-t\mathbf{A}}\mathbf{A}^\alpha \subseteq \mathbf{A}^\alpha e^{-t\mathbf{A}}$ *for all* $t > 0$.

Proof. By Theorem 3.10, $\mathbf{A}$ is the infinitesimal generator of the linear strongly continuous semigroup $\{e^{-t\mathbf{A}}\}$. Since $\mathbf{A}$ possesses a complete orthonormal system of eigenvectors, Lemma 3.4 is satisfied. Thus we have

$$\begin{aligned} \mathbf{A}^\alpha u &= \sum_n \lambda_n^\alpha \langle u_n, u\rangle u_n \\ e^{-t\mathbf{A}}u &= \sum_n e^{-t\lambda_n}\langle u_n, u\rangle u_n. \end{aligned}$$

To show the first inequality, let $t > 0$ and $u \in D(\mathbf{A}^\alpha)$.

$$\begin{aligned}
\|(e^{-t\mathbf{A}} - \mathbf{I})u\| &= \|\sum_n e^{-t\lambda_n}\langle u_n, u\rangle u_n - \sum_n \langle u_n, u\rangle u_n\| \\
&= \|\sum_n (e^{-t\lambda_n} - 1)\langle u_n, u\rangle u_n\| \\
&= \|\sum_n \frac{e^{-t\lambda_n} - 1}{(t\lambda_n)^\alpha}(t\lambda_n)^\alpha \langle u_n, u\rangle u_n\|
\end{aligned}$$

The function $\dfrac{e^{-x} - 1}{x^\alpha}$ is bounded for $x > 0$ and $0 < \alpha < 1$. Thus,

$$\|(e^{-t\mathbf{A}} - \mathbf{I})u\| \leq \|Ct^\alpha \sum_n \lambda_n^\alpha \langle u_n, u\rangle u_n\| = Ct^\alpha \|\mathbf{A}^\alpha u\|.$$

To show the second inequality, let $t > 0$. Then,

$$\begin{aligned}
\|\mathbf{A}^\alpha e^{-t\mathbf{A}}\| &= \sup_{u \in D(\mathbf{A}^\alpha)} \frac{\|\mathbf{A}^\alpha e^{-t\mathbf{A}} u\|}{\|u\|} = \sup_{u \in D(\mathbf{A}^\alpha)} \frac{\|\sum_n \lambda_n^\alpha e^{-t\lambda_n}\langle u_n, u\rangle u_n\|}{\|u\|} \\
&= \sup_{u \in D(\mathbf{A}^\alpha)} \frac{\|\sum_n t^{-\alpha}(t\lambda^n)^\alpha e^{-t\lambda_n}\langle u_n, u\rangle u_n\|}{\|u\|}.
\end{aligned}$$

The function $x^\alpha e^{-x}$ is bounded for $x > 0$ and $0 < \alpha < 1$. Thus

$$\|\mathbf{A}^\alpha e^{-t\mathbf{A}}\| \leq \sup_{u \in D(\mathbf{A}^\alpha)} \frac{Ct^{-\alpha}\|\sum_n \langle u_n, u\rangle u_n\|}{\|u\|} \leq Ct^{-\alpha}.$$

Finally, for $u \in D(\mathbf{A}^\alpha)$,

$$e^{-t\mathbf{A}}\mathbf{A}^\alpha u = \sum_n e^{-t\lambda_n}\lambda_n^\alpha \langle u_n, u\rangle u_n = \mathbf{A}^\alpha e^{-t\mathbf{A}} u.$$

Therefore $e^{-t\mathbf{A}}\mathbf{A}^\alpha \subseteq \mathbf{A}^\alpha e^{-t\mathbf{A}}$. ■

3.2.3 Initial value problems

We begin with the definition of a sectorial operator.

Definition 3.13 *The operator $\mathbf{A} : D(\mathbf{A}) \subset X \to X$ on the complex Banach space X is called sectorial if and only if the following are true:*

1. *$\mathbf{A}$ is linear, graph closed and densely defined in X.*

2. *There exists numbers $s \in \mathbb{R}, M \geq 1,$ and $\gamma \in (0, \frac{\pi}{2})$ such that the open sector*

$$\Sigma = \{\lambda \in \mathbb{C} : \gamma < |\arg(\lambda - s)| \leq \pi, \lambda \neq s\}$$

is a subset of the resolvent set of $\mathbf{A}$ *and*

$$\|(\lambda \mathbf{I} - \mathbf{A})^{-1}\| \leq M|\lambda - s|^{-1}$$

for all $\lambda \in \Sigma$.

In order to proceed with the existence theory we must show that a self-adjoint, densely defined and monotone operator on a separable Hilbert space with a complete orthonormal system of eigenvectors is sectorial.

Lemma 3.14 *Let* $\mathbf{A}$ *be a self-adjoint, densely defined and monotone operator on a separable Hilbert space,* X*. Suppose* $\mathbf{A}$ *possesses a complete orthonormal system of eigenvectors* $\{u_n\}$ *in* X*. Then* $\mathbf{A}$ *is sectorial.*

Proof. Since $\mathbf{A}$ is a self-adjoint, monotone and densely defined operator on a separable Hilbert space, $\mathbf{A}$ is linear and graph closed. Let $s = 0$, $\gamma \in (0, \frac{\pi}{2})$ and $M = \dfrac{1}{\sin(\gamma)}$. By Lemma 3.4 we have

$$\mathbf{A}u = \sum_n \lambda_n \langle u_n, u \rangle u_n$$

for $u \in D(\mathbf{A})$. Since $\mathbf{A}$ is monotone and self-adjoint, the eigenvalues of $\mathbf{A}$, λ_n, are real and positive, that is, the spectrum of $\mathbf{A}$ lies on the positive real line in the complex plane. Therefore, the set

$$\Sigma = \{\lambda \in \mathbb{C} : \gamma < |\arg(\lambda)| \leq \pi, \lambda \neq 0\}$$

is a subset of the resolvent set of $\mathbf{A}$. Let $\lambda \in \Sigma$. Then

$$|\lambda - \lambda_n| \geq Im\lambda = |\lambda| \sin(\arg(\lambda)) \geq |\lambda| \sin(\gamma).$$

Since Σ is a subset of the resolvent set of $\mathbf{A}$, $(\lambda \mathbf{I} - \mathbf{A})^{-1}$ exists. Let $v \in D(\lambda \mathbf{I} - \mathbf{A})$

$$\begin{aligned}
\|(\lambda \mathbf{I} - \mathbf{A})v\|^2 &= \|\lambda \sum_n \langle u_n, v \rangle u_n - \sum_n \lambda_n \langle u_n, v \rangle u_n\|^2 \\
&= \|\sum_n (\lambda - \lambda_n) \langle u_n, v \rangle u_n\|^2 \\
&= \sum_n |\lambda - \lambda_n|^2 \langle u_n, v \rangle^2 \langle u_n, u_n \rangle \\
&\geq \sin^2(\gamma)|\lambda|^2 \sum_n \langle u_n, v \rangle^2 \langle u_n, u_n \rangle \\
&= \sin^2(\gamma)|\lambda|^2 \|v\|^2
\end{aligned}$$

Thus, for $\lambda \in \Sigma$,

$$\begin{aligned}\|(\lambda\mathbf{I}-\mathbf{A})^{-1}\| &= \sup_{u\in D((\lambda\mathbf{I}-\mathbf{A})^{-1})} \frac{\|(\lambda\mathbf{I}-\mathbf{A})^{-1}u\|}{\|u\|} \\ &= \sup_{v\in D(\lambda\mathbf{I}-\mathbf{A})} \frac{\|v\|}{\|(\lambda\mathbf{I}-\mathbf{A})v\|} \\ &\leq \sup_{v\in D(\lambda\mathbf{I}-\mathbf{A})} \frac{\|v\|}{\sin(\gamma)|\lambda|\|v\|} \\ &\leq \frac{1}{\sin(\gamma)|\lambda|} = M|\lambda|^{-1}\end{aligned}$$

Therefore $\mathbf{A}$ is sectorial. ■

The Friedrich extension, $-\mathbf{\Delta}_F$, of $-\mathbf{\Delta}$ in Example 3.8 is sectorial by Lemma 3.14 since $-\mathbf{\Delta}_F$ is self-adjoint, monotone and densely defined with a complete orthonormal system of eigenvectors on $L^2(\Omega)$.

We continue by defining the space $C^k([a,b];X)$. A function $u(t,\mathbf{x})$ is in the space $C^k([a,b];X)$ if u is k-times continuously differentiable in t and, for any $t \in [a,b]$,

$$\frac{\partial^j u(t,\cdot)}{\partial t^j} \in X,\ j = 0,\cdots,k.$$

The norm associated with the space $C^k([a,b];X)$ is defined by

$$\|u\| = \sum_{j=0}^{k} \max_{t\in[a,b]} \|\frac{\partial^j u(t,\cdot)}{\partial t^j}\|_X.$$

Example 3.15 The space $C^1([t_0,t_1];L^2(\Omega)) = \{u(t,x)|t \to u(t,\cdot) \in L^2(\Omega)$ and $t \to u_t(t,\cdot) \in L^2(\Omega)$ are continuous on $[t_0,t_1]\}$ and has the following norm:

$$\|u\| = \max_{t\in[t_0,t_1]} \|u\|_{L^2(\Omega)} + \max_{t\in[t_0,t_1]} \|u_t\|_{L^2(\Omega)}.$$

We use the notation $u(t)\tilde{=}u(t,\cdot)$ to consider the semilinear initial value problem

$$\begin{aligned} u'(t) + \mathbf{A}u(t) &= f(t,u(t)) \quad t \in (t_0,t_1) &\quad (3.6)\\ u(t_0) &= u_0 &\quad (3.7)\end{aligned}$$

where $\mathbf{A} : D(\mathbf{A}) \subset X \to X$ is linear, densely defined, self-adjoint and strongly monotone operator, $f : \mathbb{R} \times X^\alpha \to X$ where $0 < \alpha < 1$ and $t_0 < t_1$. Our goal is to find a solution to the above initial value problem. We use the definitions for mild and strong solutions given by Henry [68] which, although slightly different than the conventional definitions, best suit our application. In the following definitions, we assume that $\mathbf{A}$ is sectorial and the space $X^\alpha = D(\mathbf{A}^\alpha)$ with the graph norm $\|x\|_\alpha = \|\mathbf{A}^\alpha x\|_X$ is defined for $\alpha > 0$. By Theorem 3.10, $-\mathbf{A}$ generates a linear strongly continuous semigroup, $\{S(t)\}$ and $u_0 \in X^\alpha$. We define a mild solution in terms of the semigroup $\{S(t)\}$.

Definition 3.16 *We say $u \in C([t_0, t_1]; X^\alpha)$ is a mild solution of the initial value problem (3.6) and (3.7) if u is a solution of the integral equation*

$$u(t) = S(t - t_0)u_0 + \int_{t_0}^{t} S(t - s)f(s, u(s))\, ds. \tag{3.8}$$

Definition 3.17 *We say u is a* strong *solution of the initial value problem (3.6) and (3.7) if u satisfies the following.*

1. *$u \in C([t_0, t_1); X^\alpha)$.*
2. *$u(t) \in D(\mathbf{A})$ for $t \in (t_0, t_1)$.*
3. *$u_t(t)$ exists for $t \in (t_0, t_1)$.*
4. *$t \to f(t, u(t)) \in X$ is locally Hölder continuous for $t \in (t_0, t_1)$, that is, there exists $0 \le \beta < 1$, such that for s, t in some bounded subset of $\mathbb{R}$ and for some constant $c > 0$.*
$$\|f(s, u(s)) - f(t, u(t))\|_X \le c|s - t|^\beta.$$
5. *$\displaystyle\int_{t_0}^{t_0+\rho} \|f(t, u(t))\|_X dt < \infty$ for some $\rho > 0$.*
6. *u satisfies equations (3.6) and (3.7).*

Definition 3.18 *We say u is a classical solution of the initial value problem (3.6) and (3.7) if*

$$u \in C^1([t_0, t_1); X) \cap C((t_0, t_1); D(A)),$$

where $D(A)$ is equipped with the graph norm, and u satisfies equations (3.6) and (3.7).

3.3 Existence theory

Let X be a Hilbert space with norm $\|\cdot\|_X$ induced by the inner product $\langle\cdot,\cdot\rangle_X$. Our goal is to find a classical solution to the initial value problem

$$u'(t) + \mathbf{A}u(t) = f(t, u(t)) \quad t \in (t_0, t_1) \tag{3.9}$$
$$u(t_0) = u_0. \tag{3.10}$$

We assume the following about the operator $\mathbf{A}$.

Hypothesis 3.19 *The operator, $\mathbf{A} : D(\mathbf{A}) \subset X \to X$, is linear, densely defined, self-adjoint, strongly monotone and possesses a complete system of eigenvectors.*

We also assume the following about the nonlinear function f.

Hypothesis 3.20 *There exists $\alpha \in [0,1), L > 0$ and $0 < \beta \leq 1$ such that*

$$\|f(t,u) - f(s,v)\|_X \leq L(|t-s|^\beta + \|u-v\|_\alpha) \tag{3.11}$$

for all $(t,u),(s,v)$ in a neighborhood of (t_0,u_0) defined by the set

$$N_\delta(t_0,u_0) = \{(x,y) \in \mathbb{R} \times X^\alpha : |x-t_0| + \|y-u_0\|_\alpha < \delta\}$$

for some $\delta > 0$.

We now state the following existence result for a mild solution.

Theorem 3.21 *(Existence and Uniqueness of Solution)*
Suppose that Hypotheses 3.19 and 3.20 hold. Then there exists $T > 0, r > 0$ such that the initial value problem (3.9) and (3.10) has exactly one mild solution $u \in Y = C([t_0,t_0+T];X^\alpha)$ with $\|u-u_0\|_Y \leq r$. Here $\|u\|_Y := \max_{t\in[t_0,t_0+T]} \|u\|_\alpha$.

The proof of a general version of Theorem 3.21 can be found in [96, pp. 171-3].
Proof. Without loss of generality, set $t_0 = 0$. Let $u_0 \in D(\mathbf{A}^\alpha)$ and $M_r = \{u \in Y : \|u-u_0\|_Y \leq r\}$ for some $r > 0$. By Theorem 3.10, $\mathbf{A}$ is the infinitesimal generator of the semigroup $\{e^{-\mathbf{A}t}\}$. Thus, our problem may be rephrased as an integral equation,

$$u(t) = e^{-\mathbf{A}t}u_0 + \int_0^t e^{-\mathbf{A}(t-s)} f(s,u(s))ds. \tag{3.12}$$

We use the contraction mapping theorem to show the existence of a fixed point of the equation

$$u = Ku, \qquad u \in M_r, \tag{3.13}$$

for some $r > 0$. Here K is a nonlinear operator defined by

$$(Ku)(t) = e^{-\mathbf{A}t}u_0 + \int_0^t e^{-\mathbf{A}(t-s)} f(s,u(s))ds.$$

First we wish to show K is a contraction mapping. Let $t > 0$ and let $u, v \in M_r$. Using the Lipschitz condition from Hypothesis 3.20, we have

$$\begin{aligned} \|(Ku)(t) - (Kv)(t)\|_\alpha &= \|\mathbf{A}^\alpha \int_0^t e^{-\mathbf{A}(t-s)}(f(s,u(s)) - f(s,v(s)))ds\| \\ &\leq \int_0^t \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}(f(s,u(s)) - f(s,v(s)))\|ds \\ &\leq \int_0^t \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}\| \; \|(f(s,u(s)) - f(s,v(s)))\|ds \\ &\leq \int_0^t \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}\|dsL\|u-v\|_\alpha. \end{aligned} \tag{3.14}$$

By Theorem 3.12 we have

$$\|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}\| \leq C(t-s)^{-\alpha} \tag{3.15}$$

where $C > 0$ depends only on α. Thus

$$\|(Ku)(t) - (Kv)(t)\|_\alpha \leq \frac{C}{1-\alpha}(t-s)^{1-\alpha} L\|u-v\|_\alpha.$$

Therefore, there exists $t_1 > 0$ such that $0 < \tilde{C}(t-s)^{1-\alpha}L < 1$ and K is a contraction for $0 \leq t \leq t_1$.

Next we wish to show that, for some $t > 0$, there exists an $r > 0$ such that K maps M_r into itself. Now,

$$\|(Ku)(t) - u_0\|_\alpha \leq \|(Ku)(t) - (Ku_0)(t)\|_\alpha + \|(Ku_0)(t) - u_0\|_\alpha.$$

Using the bound in (3.14) we have

$$\begin{aligned}
\|(Ku)(t) - u_0\|_\alpha &= \|\mathbf{A}^\alpha \int_0^t e^{\mathbf{A}(t-s)}(f(s,u(s)) - f(s,u_0(s)))ds\| + \|\mathbf{A}^\alpha(e^{\mathbf{A}t} - \mathbf{I})u_0 \\
&\quad + \mathbf{A}^\alpha \int_0^t e^{\mathbf{A}(t-s)} f(s,u_0)(s)ds\| \\
&\leq \int_0^t \|\mathbf{A}^\alpha e^{\mathbf{A}(t-s)}\| \, \|f(s,u(s)) - f(s,u_0(s)))\|ds + \|\mathbf{A}^\alpha(e^{\mathbf{A}t} - \mathbf{I})u_0\| \\
&\quad + \int_0^t \|\mathbf{A}^\alpha e^{\mathbf{A}(t-s)}\| \, \|f(s,u_0(s))\|ds \\
&\leq \int_0^t \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}\|ds(L\|u-u_0\|_\alpha + F) + \|\mathbf{A}^\alpha(e^{-\mathbf{A}t} - \mathbf{I})u_0\|
\end{aligned} \tag{3.16}$$

where $\|f(t,u_0)\| \leq F$ on $[0,t^*]$ for some $t^* > 0$. By Theorem 3.12, we have

$$\|\mathbf{A}^\alpha(e^{-\mathbf{A}t} - \mathbf{I})u_0\| = \|(e^{-\mathbf{A}t} - \mathbf{I})\mathbf{A}^\alpha u_0\|. \tag{3.17}$$

since $u_0 \in D(\mathbf{A}^\alpha)$. Applying (3.15) and (3.17) to (3.16), we have

$$\begin{aligned}
\|(Ku)(t) - u_0\|_\alpha &\leq \int_0^t C(t-s)^{-\alpha}ds(L\|u-u_0\|_\alpha + F) + \|(e^{-\mathbf{A}t} - \mathbf{I})\mathbf{A}^\alpha u_0\| \\
&= \frac{Ct^{1-\alpha}}{1-\alpha}(L\|u-u_0\|_\alpha + F) + \|(e^{-\mathbf{A}t} - \mathbf{I})\mathbf{A}^\alpha u_0\|.
\end{aligned} \tag{3.18}$$

The right hand side of (3.18) can be written as $z(t)\|u-u_0\|_\alpha + v(t)$. We need only to show $z(t) \to 0$ and $v(t) \to 0$ as $t \to 0^+$. Since $u_0 \in D(\mathbf{A}^\alpha)$ and $\{e^{-\mathbf{A}t}\}$ is a strongly continuous semigroup, we have

$$e^{-\mathbf{A}(t)}\mathbf{A}^\alpha u_0 - \mathbf{A}^\alpha u_0 \to 0$$

as $t \to 0^+$. Also, $\dfrac{Ct^{1-\alpha}}{1-\alpha} \to 0$ as $t \to 0$. Thus there exist $r > 0$ and $t_2 > 0$ such that

$$\|(Ku)(t) - u_0\|_\alpha \leq C(t_2)\|u-u_0\|_\alpha \leq r$$

Thus, we have shown $K(M_r) \subset M_r$. Upon setting $T = \min\{t_1, t_2\}$, the contraction mapping theorem ensures the existence of a unique solution to (3.13). ■

Once we obtain a mild solution of the initial value problem (3.9) and (3.10), we apply the following theorem to ensure the solution is a strong solution. Let $t_1 = t_0 + T$.

Theorem 3.22 *Let* $\mathbf{A}$ *be the infinitesimal generator of a* c_0*-semigroup* $\{\mathbf{S}(t)\} = \{e^{-\mathbf{A}t}\}$*. Suppose Hypothesis 3.20 holds. If* $u \in C([t_0, t_1]; X^\alpha)$ *is a mild solution of the initial value problem (3.9) and (3.10) and*

$$\int_{t_0}^{t_0+\rho} \|f(t, u(t))\|_X dt < \infty$$

for some $\rho > 0$*, then* u *is a strong solution of the initial value problem (3.9) and (3.10).*

In order to prove Theorem 3.22, we need the following lemma.

Lemma 3.23 *Let* $f : (0, T) \to X$ *be locally Hölder continuous with* $\int_0^\rho \|f(t)\| ds < \infty$ *for some* $\rho > 0$*. For* $0 \le t < T$*, define*

$$F(t) := \int_0^t e^{-\mathbf{A}(t-s)} f(s) ds.$$

Then $F(\cdot)$ *is continuous on* $[0, T)$*, continuously differentiable on* $(0, T)$*, with* $F(t) \in D(\mathbf{A})$ *for* $t \in (0, T)$*,* $F_t(t) + \mathbf{A}F(t) = f(t)$ *on* $(0, T), and F(t) \to 0$ *in* X *as* $t \to 0^+$*.*

Proof. First we show that F is continuous from $[0, T)$ onto X. For small $\rho > 0$, define

$$F_\rho(t) := \int_0^{t-\rho} e^{-\mathbf{A}(t-s)} f(s) ds, \quad \rho \le t < T,$$

with $F_\rho(t) = 0$ for $0 \le t \le \rho$. Then, setting $f(s) = 0$ for $s < 0$,

$$\|F(t) - F_\rho(t)\| \le \int_{t-\rho}^t \|e^{-\mathbf{A}(t-s)}\| \, \|f(s)\| ds$$

which tends to 0 as $\rho \to 0^+$, uniformly on $[0, t_0]$ for any $t_0 < T$. Also, $F_\rho(t)$ is continuous, since, for $0 \le t \le t + h \le t_0$,

$$F_\rho(t+h) - F_\rho(t) = (e^{-\mathbf{A}h} - \mathbf{I}) \int_0^{t-\rho} e^{-\mathbf{A}(t-s)} f(s) ds + \int_{t-\rho}^{t+h-\rho} e^{-\mathbf{A}(t+h-s)} f(s) ds,$$

which tends to 0 as $h \to 0$. Therefore F is continuous on $[0, T)$ into X, and

$$\|F(t)\| \le \int_0^t \|e^{-\mathbf{A}(t-s)}\| \, \|f(s)\| ds \to 0$$

as $t \to 0^+$.

Next we show $F(t) \in D(\mathbf{A})$. If $0 \leq s < t$, then $e^{-\mathbf{A}(t-s)} f(s) \in D(\mathbf{A})$, so the Riemann sums for $F_\rho(t)$,

$$\sum_{t-s_j \geq \rho} e^{-\mathbf{A}(t-s_j)} f(s_j) \Delta s_j,$$

are in $D(\mathbf{A})$, and

$$\lim_{\Delta s \to 0} \mathbf{A} \sum_{s \leq t-\rho} e^{-\mathbf{A}(t-s)} f(s) \Delta s = \int_0^{t-\rho} \mathbf{A} e^{-\mathbf{A}(t-s)} f(s) ds.$$

Thus, since $\mathbf{A}$ is closed, $F_\rho(t) \in D(\mathbf{A})$ and

$$\mathbf{A} F_\rho(t) = \int_0^{t-\rho} \mathbf{A} e^{-\mathbf{A}(t-s)} f(s) ds = \int_0^{t-\rho} \mathbf{A} e^{-\mathbf{A}(t-s)} (f(s) - f(t)) ds + (e^{-\mathbf{A}\rho} - e^{-\mathbf{A}t}) f(t).$$

Now $\|\mathbf{A} e^{\mathbf{A}(t-s)}\| = O((t-s)^{-1})$ and $\|f(s) - f(t)\| = O(|t-s|^\theta)$ for some $\theta > 0$ as $s \to t^-$, hence, as $\rho \to 0^+$,

$$\mathbf{A} F_\rho(t) \to \int_0^t \mathbf{A} e^{-\mathbf{A}(t-s)} (f(s) - f(t)) ds + (\mathbf{I} - e^{-\mathbf{A}t}) f(t).$$

Thus, again since $\mathbf{A}$ is closed, $F(t) \in D(\mathbf{A})$ for $0 < t < T$.

Now, consider any interval $[t_0, t_1] \subset (0, T)$. Then $\mathbf{A} F_\rho(t) \to \mathbf{A} F(t)$ uniformly on $[t_0, t_1]$ since, by hypothesis, $\|f(t) - f(s)\| \leq K|t-s|^\theta$ for $t, s \in [t_0, t_1]$ and some $\theta > 0$, so

$$\begin{aligned}
\|\mathbf{A} F_\rho(t) - \mathbf{A} F(t)\| &= \|(-\mathbf{I} + e^{-\mathbf{A}\rho}) f(t) + \int_{t-\rho}^t \mathbf{A} e^{-\mathbf{A}(t-s)} (f(s) - f(t)) ds\| \\
&\leq \|(e^{-\mathbf{A}\rho} - \mathbf{I}) f(t)\| + C \int_{t-\rho}^t (t-s)^{-1+\theta} ds \to 0
\end{aligned}$$

as $\rho \to 0^+$, uniformly on $[t_0, t_1]$.

Finally, we show $F(t)$ is differentiable. $F_\rho(t)$ is differentiable when $t > \rho$, with

$$\frac{dF_\rho(t)}{dt} = -\mathbf{A}_\rho(t) + e^{-\mathbf{A}\rho} f(t-\rho), \quad \rho < t < T.$$

The right side of the above equation converges uniformly to $-\mathbf{A}F(t) + f(t)$ on $[t_0, t_1] \subset (0, T)$ as $\rho \to 0^+$, so F is continuously differentiable on $(0, T)$, with $F_t(t) + \mathbf{A}F(t) = f(t)$. ■

We now proceed with the proof of Theorem 3.22.

Proof. We note that criterion (1) of Definition 3.17, the definition of a strong solution, is satisfied since u is a mild solution. Also, by hypothesis, criterion (5) of Definition 3.17 is satisfied. Thus it remains to be shown that (2)-(4) and (6) of Definition 3.17 hold.

Again, we set $t_0 = 0$. From Hypothesis 3.20, we know that $f(t,u)$ is locally Hölder continuous in t and locally Lipschitz continuous in u. Thus to show (4), we need only to show that $t \to u(t) \in D(\mathbf{A})$ is locally Hölder continuous on $(0,T)$. Since u is a mild solution of (3.9) and (3.10), u satisfies the integral equation (3.12). Let $t \in [t_0, t_1] \subset (0,T)$ and let $h > 0$ be such that $t_0 \leq t < t+h \leq t_1$. Then,

$$\begin{aligned} \|u(t+h) - u(t)\|_\alpha &= \|(e^{-\mathbf{A}h} - \mathbf{I})e^{-\mathbf{A}t}u_0 + \int_0^t (e^{-\mathbf{A}h} - \mathbf{I})e^{-\mathbf{A}(t-s)} f(s,u(s))ds \\ &\quad + \int_t^{t+h} e^{-\mathbf{A}(t+h-s)} f(s,u(s))ds\|_\alpha. \end{aligned}$$

Now, by Theorem 3.12, since u_0 and $e^{-\mathbf{A}(t-s)}f \in D(\mathbf{A}^\alpha)$, we have

$$\begin{aligned} \|u(t+h) - u(t)\|_\alpha &\leq \|\mathbf{A}^\alpha e^{-\mathbf{A}t}\| \; \|(e^{-\mathbf{A}h} - \mathbf{I})u_0\| \\ &\quad + \int_0^t \|\mathbf{A}^\alpha\| \; \|(e^{-\mathbf{A}h} - \mathbf{I})e^{-\mathbf{A}(t-s)} f(s,u(s))\| ds \\ &\quad + \int_t^{t+h} \|\mathbf{A}^\alpha e^{-\mathbf{A}(t+h-s)}\| \; \|f(s,u(s))\| ds \\ &\leq Ch^\alpha t^{-\alpha}\|u_0\|_\alpha + \int_0^t Ch^\alpha \|\mathbf{A}^\alpha\| \; \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}\| \; \|f(s,u(s))\| ds \\ &\quad + \int_t^{t+h} C(t+h-s)^\alpha \|f(s,u(s))\| ds \\ &\leq Ch^\alpha t^{-\alpha}\|u_0\|_\alpha + \int_0^t C(t-s)^{-\alpha} h^\alpha \|f(s,u(s))\| ds \\ &\quad + \int_t^{t+h} C(t+h-s)^\alpha \|f(s,u(s))\| ds \\ &= Ch^\alpha \end{aligned}$$

since $t^{-\alpha}$ is bounded for $t \in [t_0^*, t_1^*]$. Thus, $t \to u(t)$ is locally Hölder continuous on $(0,T)$ into X^α which, in turn, implies $t \to f(t,u(t))$ is locally Hölder continuous on $(0,T)$ into X.

Now let $f(t) := f(t,u(t))$. Since $t \to f(t,u(t))$ is locally Hölder continuous on $(0,T)$ into X, $t \to f(t,)$ is also locally Hölder continuous on $(0,T)$ into X. Then, by Lemma 3.23,

$$F(t) = \int_0^t \mathbf{T}(t-s)f(s)ds \in D(\mathbf{A})$$

for $t \in (0,T)$. This, in turn, implies $u(t) \in D(\mathbf{A})$ since $e^{-\mathbf{A}t}u_0 \in D(\mathbf{A})$ by Theorem 3.11. Thus (2) holds.

Note that since $f : (0,T) \to X$ is locally Hölder continuous with $\int_0^\rho \|f(s)\|_X < \infty$ for some $\rho > 0$, Lemma 3.23 implies that (3) holds, so we need only show (6). Since

$F(0) = 0$ and $u(t) = \mathbf{T}(t)u_0 + F(t)$, we have

$$u_t(t) = \frac{\partial \mathbf{T}(t)u_0}{\partial t} + F_t(t) = \mathbf{A}\mathbf{T}(t)u_0 + \mathbf{A}F(t) + f(t) = \mathbf{A}(\mathbf{T}(t)u_0 + F(t)) + f(t) = \mathbf{A}u(t) + f(t)$$

by Theorem 3.11. We also have

$$u(0) = \mathbf{T}(0)u_0 + F(0) = u_0.$$

Thus u is the solution of

$$\begin{aligned} y_t &= \mathbf{A}y + f(t) \\ y(0) &= u_0 \end{aligned}$$

and is, therefore, a solution of the initial value problem (3.9) and (3.10). ■

In order to obtain a classical solution to the initial value problem (3.9) and (3.10) we need the following theorem.

Theorem 3.24 *Assume* $\mathbf{A}$ *is sectorial and* $f : U \to X$ *is locally Lipschitz continuous on an open set* $U \subset \mathbb{R} \times X^\alpha$, *for some* $0 \le \alpha < 1$ *and* $(0, u_0) \in U$. *Suppose* u *is a strong solution of the initial value problem (3.6) and (3.10). Then, if* $\gamma < 1$, $u_t \in C((t_0, t_1); X^\gamma)$ *with*

$$\|u_t\|_\gamma \le Ct^{\alpha-\gamma-1}. \tag{3.19}$$

In order to prove Theorem 3.24 we need the following lemma.

Lemma 3.25 *Suppose* $\mathbf{A}$ *is sectorial,* $f : (0, T) \to X$ *satisfies* $\|f(t) - f(s)\| \le K(s)(t-s)^\gamma$ *for* $0 < \gamma < 1$, *and* $0 < s < t < T < \infty$, *where* $K(\cdot)$ *is continuous on* $(0, T)$ *and* $\int_0^T K(s)ds < \infty$. *Then* $F(t) := \int_0^t e^{-\mathbf{A}(t-s)} f(s)ds, 0 < t < T$, *is continuously differentiable on* $(0, T)$ *into* X^β, *provided* $0 \le \beta < \gamma$, *and*

$$\|F_t\|_\beta \le Mt^{-\beta}(\|f(t)\| + \int_0^t (t-s)^{\gamma-\beta-1} K(s)ds$$

for $0 < t < T$, *where* $M > 0$ *is independent of* γ, β *and* $f(\cdot)$. *Furthermore, if* $\int_0^h K(s)ds = O(h^\delta)$ *as* $h \to 0^+$, *then* $t \to F_t$ *is locally Hölder continuous from* $(0, T)$ *to* X^β *for some* $\delta > 0$.

Proof. We present the proof for $\beta = 0$. The proof for $0 < \beta < \gamma$ is similar. Since K is continuous on $(0, T)$ and $\int_0^T K(s)ds < \infty$, K is bounded on $(0, T)$. Thus F is Hölder continuous. Then by Lemma 3.23, we have

$$F_t(t) = e^{-\mathbf{A}t} f(t) + \int_0^t \mathbf{A} e^{-\mathbf{A}(t-s)} (f(t) - f(s)) ds.$$

Thus, for $t \in (0, T)$,

$$\begin{aligned}
\|u_t(t)\| &\leq \| - \mathbf{A} e^{-\mathbf{A}t} u_0\| + \|e^{-\mathbf{A}t} f(t)\| + \int_0^t \|e^{-\mathbf{A}(t-s)} (f(t) - f(s))\| ds \\
&\leq C\|u_0\| + \|e^{-\mathbf{A}t} f(t)\| + C \int_0^t (t-s)^{\gamma-1} \|f(t) - f(s)\| ds \\
&\leq M\|f(t)\| + M \int_0^t (t-s)^{\gamma-1} K(s) ds.
\end{aligned}$$

■

We now proceed with the proof of Theorem 3.24.

Proof. Again, we present the proof for $\beta = 0$. The proof for $0 < \beta < \gamma$ is similar. Let $t_0 = 0$. Since u is a mild solution of of the initial value problem (3.6) and (3.10),

$$u = e^{-\mathbf{A}t} u_0 + \int_0^t e^{-\mathbf{A}(t-s)} f(s, u(s)) ds.$$

Since

$$\frac{d}{dt} e^{-\mathbf{A}t} u_0 = \mathbf{A} e^{-\mathbf{A}t} u_0$$

is continuous on $(0, T)$, we need to show that

$$\frac{d}{dt} \int_0^t e^{-\mathbf{A}(t-s)} f(s, u(s)) ds$$

exists and is continuous on $(0, T)$.

Let $\alpha < \beta < 1, 0 < \tau < T$. Then $\|u(\tau)\|_\beta \leq C_1 \tau^{\alpha-\beta}$ and $g(t) := f(t, u(t))$ satisfies

$$\|g(t) - g(s)\| \leq L(|t-s|) + \|u(t) - u(s)\|_\alpha)$$

for $0 \leq s \leq t \leq T$, for some $L > 0$ and $C_1 > 0$.

We wish to apply Lemma 3.25 to

$$\int_0^t e^{-\mathbf{A}(t-s)} g(s) ds.$$

For $\tau < t < t+h \leq T$,

$$\begin{aligned} u(t+h) - u(t) &= (e^{-\mathbf{A}h} - \mathbf{I})e^{-\mathbf{A}(t-\tau)}u(\tau) + \int_\tau^{\tau+h} e^{-\mathbf{A}(t+h-s)}g(s)ds \\ &\quad + \int_{\tau+h}^{t+h} e^{-\mathbf{A}(t+h-s)}g(s)ds - \int_\tau^t e^{-\mathbf{A}(t-s)}g(s)ds \\ &= (e^{-\mathbf{A}h} - \mathbf{I})e^{-\mathbf{A}(t-\tau)}u(\tau) + \int_\tau^t e^{-\mathbf{A}(t-s)}\{g(s+h) - g(s)\}ds \\ &\quad + \int_\tau^{\tau+h} e^{-\mathbf{A}(t+h-s)}g(s)ds. \end{aligned}$$

Thus

$$\begin{aligned} \|u(t+h) - u(t)\|_\alpha &\leq \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-\tau)}\| \; \|(e^{-\mathbf{A}h} - \mathbf{I})u(\tau)\| \\ &\quad + \int_\tau^t \|\mathbf{A}^\alpha e^{-\mathbf{A}(t-s)}\| \; \|g(s+h) - g(s)\|ds \\ &\quad + \int_\tau^{\tau+h} \|\mathbf{A}^\alpha e^{-\mathbf{A}(t+h-s)}\| \; \|g(s)\|ds. \end{aligned}$$

Let $0 < \alpha < \beta < 1$. Then for $t \in (\tau, \tau+h)$ and h small, we have, by Theorem 3.12,

$$\|\mathbf{A}^\alpha e^{-\mathbf{A}(t-\tau)}\| \; \|(e^{-\mathbf{A}h} - \mathbf{I})u(\tau)\| \leq C(t-\tau)^{-\alpha}h^\beta\|u(\tau)\|_\beta \leq Ch(t-\tau)^{-1+\beta-\alpha}\|u(\tau)\|_\beta. \quad (3.20)$$

Also, since $(t+h-s)^{-\alpha} \leq (t-\tau)^{-\alpha}$ on the interval $(\tau, \tau+h)$ for small h, we have

$$\begin{aligned} \int_\tau^{\tau+h} \|\mathbf{A}^\alpha e^{\mathbf{A}(t+h-s)}\| \; \|g(s)\|ds &\leq \int_\tau^{\tau+h} C(t+h-s)^{-\alpha}\|g(s)\|ds \\ &\leq C(t-\tau)^{-\alpha}\int_\tau^{\tau+h} \|g(s)\|ds \leq Ch(t-\tau)^{-\alpha} \end{aligned} \quad (3.21)$$

Using the bounds obtained in (3.20) and (3.21), we have

$$\begin{aligned} \|g(t+h) - g(t)\| &\leq Lh + L\|u(t+h) - u(t)\|_\alpha \\ &\leq Lh + C_2h((t-\tau)^{-1+\beta-\alpha}\|u(\tau)\|_\beta + (t-\tau)^{-\alpha}) \\ &\quad + \int_\tau^t M(t-s)^{-\alpha}\|g(s+h) - g(s)\|ds. \end{aligned}$$

Thus, applying Gronwall's inequality,

$$\|g(t+h) - g(t)\| \leq C_3h((t-\tau)^{-1+\beta-\alpha}\|u(\tau)\|_\beta + (t-\tau)^{-\alpha}).$$

Let

$$K(t) = (t-\tau)^{-1+\beta-\alpha}\|u(\tau)\|_\beta + (t-\tau)^{-\alpha}.$$

Then K is continuous on (τ, T) and $\int_\tau^T K(t)dt < \infty$. Therefore, by Lemma 3.25, $t \to u_t$ is Hölder continuous on (τ, T) with

$$\begin{aligned}\|u_t\| &\leq C_4[(t-\tau)^{\beta-1}\|u(\tau)\|_\beta + (t-\tau)^{-1}] \\ &\leq C_5[(t-\tau)^{\beta-1}\tau^{\alpha-\beta} + (t-\tau)^{-1}].\end{aligned}$$

Now take $t = 2\tau$ so that

$$\|u_t\| \leq Mt^{\alpha-1}.$$

■

The complete proofs of Lemma 3.25 and Theorem 3.24 can be found in [68, pp. 71-2].

3.4 Proof of Theorem 3.1

Upon rewriting the initial value problem (2.44)-(2.49) with homogeneous boundary conditions, our problem becomes:
Find $t_1 > 0$ for which there exists a unique $\mathbf{u} \in C^1([0, t_1); L^2(0, l)^3) \cap C((0, t_1); [H^2(0, l) \cap H_0^1(0, l)]^3)$ such that $\mathbf{u}$ satisfies the initial value problem

$$\begin{aligned}\mathbf{u}'(t) + \mathbf{A}\mathbf{u}(t) &= \mathbf{f}(t, \mathbf{u}(t)) \quad t \in (0, t_1) &\quad (3.22)\\ \mathbf{u}(0) &= \mathbf{u}_0 \in H_0^1(0, l)^3 &\quad (3.23)\end{aligned}$$

with

$$\mathbf{u}(t) = \begin{bmatrix} w(t,x) \\ v(t,x) \\ \phi(t,x) \end{bmatrix},$$

$$\mathbf{A} = \begin{bmatrix} -\epsilon_1^2 \frac{\partial^2}{\partial x^2} & 0 & 0 \\ 0 & -\epsilon_2^2 \frac{\partial^2}{\partial x^2} & 0 \\ 0 & 0 & -\epsilon_3^2 \frac{\partial^2}{\partial x^2} \end{bmatrix} \tag{3.24}$$

and

$$\mathbf{f}(t, \mathbf{u}(t)) = \begin{bmatrix} v_x(t,x) \\ G'(w(t,x))_x - \gamma\phi_x(t,x) \\ \gamma w(t,x) - \alpha\phi(t,x) \end{bmatrix}. \tag{3.25}$$

The domain of $\mathbf{A}$ is $D(\mathbf{A}) = [H^2(0, l) \cap H_0^1(0, l)]^3$. Let $X = L^2(0, l)^3$, then $\mathbf{A}$ is closed, densely defined in X. $\mathbf{A}$ is linear by virtue of the differential operator $\frac{-\partial^2}{\partial x^2} = -\mathbf{\Delta}$ in one space dimension and strongly monotone since, for $\mathbf{u} \in D(\mathbf{A})$,

$$\langle \mathbf{A}\mathbf{u}, \mathbf{u}\rangle_{L^2} = \int_0^l -\epsilon_1^2 \frac{\partial^2 w}{\partial x^2} w - \epsilon_2^2 \frac{\partial^2 v}{\partial x^2} v - \epsilon_3^2 \frac{\partial^2 \phi}{\partial x^2} \phi \, dx$$

$$
\begin{aligned}
&= \int_0^l \epsilon_1^2 \frac{\partial w}{\partial x}\frac{\partial w}{\partial x} + \epsilon_2^2 \frac{\partial v_1}{\partial x}\frac{\partial v_1}{\partial x} + \epsilon_3^2 \frac{\partial \phi_1}{\partial x}\frac{\partial \phi_1}{\partial x}\, dx \\
&\geq \min\{\epsilon_1^2, \epsilon_2^2, \epsilon_3^2\} \int_0^l \frac{\partial w}{\partial x}\frac{\partial w}{\partial x} + \frac{\partial v}{\partial x}\frac{\partial v}{\partial x} + \frac{\partial \phi}{\partial x}\frac{\partial \phi}{\partial x}\, dx \\
&= c\langle \mathbf{u}_x, \mathbf{u}_x\rangle_{L^2}
\end{aligned}
$$

where $c = \min\{\epsilon_1^2, \epsilon_2^2, \epsilon_3^2\} > 0$, since $\epsilon_i^2 > 0, i = 1, 2, 3$. $\mathbf{A}$ is symmetric since, for $\mathbf{u}_1, \mathbf{u}_2 \in D(\mathbf{A})$,

$$
\begin{aligned}
\langle \mathbf{A}\mathbf{u}_1, \mathbf{u}_2\rangle_{L^2} &= \int_0^l -\epsilon_1^2 \frac{\partial^2 w_1}{\partial x^2} w_2 - \epsilon_2^2 \frac{\partial^2 v_1}{\partial x^2} v_2 - \epsilon_3^2 \frac{\partial^2 \phi_1}{\partial x^2} \phi_2\, dx \\
&= \int_0^l \epsilon_1^2 \frac{\partial w_1}{\partial x}\frac{\partial w_2}{\partial x} + \epsilon_2^2 \frac{\partial v_1}{\partial x}\frac{\partial v_2}{\partial x} + \epsilon_3^2 \frac{\partial \phi_1}{\partial x}\frac{\partial \phi_2}{\partial x}\, dx \\
&= \int_0^l w_1(-\epsilon_1^2 \frac{\partial^2 w_2}{\partial x^2}) + v_1(-\epsilon_2^2 \frac{\partial^2 v_2}{\partial x^2}) + \phi_1(-\epsilon_3^2 \frac{\partial^2 \phi_2}{\partial x^2})\, dx \\
&= \langle \mathbf{u}_1, \mathbf{A}\mathbf{u}_2\rangle_{L^2}.
\end{aligned}
$$

In fact, since $D(\mathbf{A}) = [H^2(0,l) \cap H_0^1(0,l)]^3$, $\mathbf{A}$ is self-adjoint. Thus, $\mathbf{A} = \mathbf{A}_F$.

Using Poincare's inequality, we have

$$
\langle \mathbf{A}\mathbf{u}, \mathbf{u}\rangle_{L^2} \geq c\langle \mathbf{u}_x, \mathbf{u}_x\rangle_{L^2} \geq \hat{c}\langle \mathbf{u}, \mathbf{u}\rangle_{L^2} = \hat{c}\|\mathbf{u}\|_{L^2}^2
$$

where $\hat{c} > 0$. The Energetic space, X_E, of the operator $\mathbf{A}$ is the completion of the domain of $\mathbf{A}$ with respect to the inner product:

$$
\langle \mathbf{u}, \mathbf{v}\rangle_E = \langle \mathbf{A}\mathbf{u}, \mathbf{v}\rangle_{L^2}
$$

for all $\mathbf{u}, \mathbf{v}$ in $D(\mathbf{A})$. Hence $X_E = H_0^1(0,l)^3$.

Since $\mathbf{A}$, is linear, densely defined, self-adjoint and strongly monotone, $\mathbf{A}$ satisfies Hypothesis 3.19 of Theorem 3.21. The energetic extension of $\mathbf{A}$, $\mathbf{A}_E$, is defined on the space $D(\mathbf{A}_E) = H_0^1(0,1)^3$. Recalling the Laplacian operator of Example 3.8, we extend equation (3.3) to the domain of $\mathbf{A}$ defined in (3.24). Thus

$$
X^{\frac{1}{2}} = H_0^1(0,l)^3.
$$

We now show that $\mathbf{f}$ satisfies Hypothesis 3.20. Since $\mathbf{f}(t, \mathbf{u})$ defined by (3.25) is solely a function of $\mathbf{u}$, we need only show $\mathbf{f}$ is locally Lipschitz continuous in $\mathbf{u}$ to satisfy the inequality (3.11). We define $N_\delta(\mathbf{v}) = \{\mathbf{u} \in H_0^1(0,l)^3 : \|\mathbf{u} - \mathbf{v}\|_{H^1} < \delta\}$ to be a bounded neighborhood of $\mathbf{v}$ in $H_0^1(0,l)^3$. Suppose $\mathbf{u} \in N_\delta(\mathbf{u}_0)$, the Sobolev Embedding Theorem gives us a uniform L^∞ bound for each of the components of $\mathbf{u}$. Moreover, since $G \in C^3(\mathbb{R})$, the composition $G^k(w), k = 0, 1, 2, 3$ is uniformly bounded in the L^∞ norm on $N_\delta(\mathbf{u}_0)$, i.e., there is a constant c_G such that

$$
\|G^k(w)\|_{L^\infty(0,l)} \leq c_G \tag{3.26}
$$

for all $w \in N_\delta(w_0) := \{w \in H_0^1(0,l) : \|w - w_0\|_{H^1(0,l)} < \delta\}$ and $k = 0, 1, 2, 3$. Thus from (3.25), we see that $\mathbf{f} : H_0^1(0,l)^3 \to L^2(0,l)^3$. Likewise, using the Mean Value Theorem, for $w_1, w_2 \in N_\delta(w_0)$, we have

$$\begin{aligned} \max_{x\in[0,l]} |G''(w_1(x)) - G''(w_2(x))| &= \max_{x\in[0,l]} (|G'''(\xi_x)||w_1(x) - w_2(x)|) \\ &\leq c_G \max_{x\in[0,l]} |w_1(x) - w_2(x)|. \end{aligned} \tag{3.27}$$

Let $\|\cdot\|_{L^2}$ and $\|\cdot\|_{H^1}$ denote the graph norms on $L^2(0,l)^3$ and $H_0^1(0,l)^3$ respectively, i.e., for $\mathbf{u} \in L^2(0,l)^3$ and $\mathbf{v} \in H_0^1(0,l)^3$

$$\|\mathbf{u}\|_{L^2} = \left(\sum_{i=1}^{3} \|u_i\|_{L^2(0,l)}^2\right)^{\frac{1}{2}}$$

and

$$\|\mathbf{v}\|_{H^1} = \left(\sum_{i=1}^{3} \|v_{ix}\|_{L^2(0,l)}^2\right)^{\frac{1}{2}}.$$

On the bounded neighborhood $N_\delta(\mathbf{u}_0)$, $\|\cdot\|_{L^2}$ and $\|\cdot\|_{H^1}$ are equivalent to the norms $\|\cdot\|_{L^2}^*$ and $\|\cdot\|_{H^1}^*$ respectively, where

$$\|\mathbf{u}\|_{L^2}^* = \sum_{i=1}^{3} \|u_i\|_{L^2(0,l)}$$

and

$$\|\mathbf{v}\|_{H^1}^* = \sum_{i=1}^{3} \|v_{ix}\|_{L^2(0,l)}$$

for $\mathbf{u} \in L^2(0,l)^3$ and $\mathbf{v} \in H_0^1(0,l)^3$.

Let $\mathbf{u}_1, \mathbf{u}_2 \in N_\delta(\mathbf{u}_0)$ for some $\delta > 0$. Then, since $\|\cdot\|_{L^2}$ is equivalent to $\|\cdot\|_{L^2}^*$,

$$\begin{aligned} \|\mathbf{f}(\mathbf{u}_1) - \mathbf{f}(\mathbf{u}_2)\|_{L^2} &\leq c(\|G''(w_1)w_{1,x} - G''(w_2)w_{2,x} - \gamma\phi_{1,x} + \gamma\phi_{2,x}\|_{L^2(0,l)} \\ &\quad + \|v_{1,x} - v_{2,x}\|_{L^2(0,l)} + \|\gamma w_1 - \gamma w_2 - \alpha\phi_1 + \alpha\phi_2\|_{L^2(0,l)}) \\ &\leq c(\max_{x\in[0,l]} |G''(w_1(x))| \|w_{1,x} - w_{2,x}\|_{L^2(0,l)} \\ &\quad + \|w_{2,x}\|_{L^2(0,l)} \|G''(w_1) - G''(w_2)\|_{L^2(0,l)} \\ &\quad + |\gamma| \|\phi_{1,x} - \phi_{2,x}\|_{L^2(0,l)} + \|v_{1,x} - v_{2,x}\|_{L^2(0,l)} \\ &\quad + |\gamma| \|w_1 - w_2\|_{L^2(0,l)} + |\alpha| \|\phi_1 - \phi_2\|_{L^2(0,l)}). \end{aligned}$$

Using (3.26) and (3.27) we have

$$\begin{aligned} \|\mathbf{f}(\mathbf{u}_1) - \mathbf{f}(\mathbf{u}_2)\|_{L^2} &\leq c(c_G \|w_{1,x} - w_{2,x}\|_{L^2(0,l)} \\ &\quad + c_G \|w_{2,x}\|_{L^2(0,l)} \|w_1 - w_2\|_{L^2(0,l)} \\ &\quad + |\gamma| \|\phi_{1,x} - \phi_{2,x}\|_{L^2(0,l)} + \|v_{1,x} - v_{2,x}\|_{L^2(0,l)} \\ &\quad + |\gamma| \|w_1 - w_2\|_{L^2(0,l)} + |\alpha| \|\phi_1 + \phi_2\|_{L^2(0,l)}). \end{aligned}$$

By the equivalence of the norms $\|u_x\|_{L^2(0,l)}$ and $\|u\|_{H^1(0,l)}$ on $H_0^1(0,l)$ and Poincare's inequality, we have

$$\begin{aligned}\|\mathbf{f}(\mathbf{u}_1)-\mathbf{f}(\mathbf{u}_2)\|_{L^2} \;&\leq\; c((c_G+c_Gc_p\|w_2\|_{H^1(0,l)}+c_p|\gamma|)\|w_1-w_2\|_{H^1(0,l)}\\ &\quad+\|v_1-v_2\|_{H^1(0,l)})+(|\gamma|+c_p|\alpha|)\|\phi_1-\phi_2\|_{H^1(0,l)})\end{aligned}$$

where $c_p>0$ is the constant due to Poincare's inequality. Since $\mathbf{u}_2\in N_\delta(\mathbf{u}_0)$,

$$\|w_2\|_{H^1(0,l)}\leq\|w_2-w_0\|_{H^1(0,l)}+\|w_0\|_{H^1(0,l)}\leq\delta+\|w_0\|_{H^1(0,l)}=\delta_{w_0}$$

and thus

$$\|\mathbf{f}(\mathbf{u}_1)-\mathbf{f}(\mathbf{u}_2)\|_{L^2}\leq c\max\{(c_G+c_Gc_p\delta_{w_0}+c_p|\gamma|),1,(|\gamma|+c_p|\alpha|)\}\|\mathbf{u}_1-\mathbf{u}_2\|^*_{H^1}.$$

Lastly, using the equivalence of between the norms $\|\cdot\|_{H^1}$ and $\|\cdot\|^*_{H^1}$,

$$\|\mathbf{f}(\mathbf{u}_1)-\mathbf{f}(\mathbf{u}_2)\|_{L^2}\leq L\|\mathbf{u}_1-\mathbf{u}_2\|_{H^1}$$

where

$$0<L=\hat{c}\max\left\{(c_G+c_Gc_p\delta_{w_0}+c_p|\gamma|),1,(|\gamma|+c_p|\alpha|)\right\}.$$

Therefore Hypothesis 3.20 is satisfied. Thus, by Theorem 3.21, we can be assured that there exists $t_1>0, r>0$ such that the initial value problem (3.22) and (3.23) has exactly one mild solution, $\bar{\mathbf{u}}\in Y=C([0,t_1);H_0^1(0,l)^3)$ with

$$\|\bar{\mathbf{u}}-\mathbf{u}_0\|_Y\leq r, \tag{3.28}$$

where $\|\mathbf{u}\|_Y=\max\limits_{t\in(0,t_1]}\|\bar{\mathbf{u}}\|_{H^1}$.

We now show that this mild solution is, in fact, a classical solution of the original initial value problem (2.44)-(2.49) with homogeneous boundary conditions. First we note that since $\mathbf{A}$ is densely defined in $L^2(0,l)^3$, self-adjoint and strongly monotone, it satisfies Lemma 3.14. Thus $\mathbf{A}$ is sectorial. By Theorem 3.10, $-\mathbf{A}$ generates a linear strongly continuous semigroup $\{S(t)\}$, and, by definition, the mild solution $\bar{\mathbf{u}}$ satisfies the integral equation (3.12).

We show that

$$\int_0^{t_1}\|f(t,\bar{\mathbf{u}}(t))\|_{L^2}dt<\infty$$

by the same argument used to show f is locally Lipschitz. Since $f(t,\mathbf{u})=f(\mathbf{u})$, we need only show $\|\mathbf{f}(\bar{\mathbf{u}}(t))\|_{L^2}$ is bounded on $(0,t_1)$ Let $t\in(0,t_1)$.

$$\begin{aligned}\|\mathbf{f}(\bar{\mathbf{u}}(t))\|_{L^2} \;&\leq\; c(\|G''(\bar{w}(t))\bar{w}_x(t)-\gamma\bar{\phi}_x(t)\|_{L^2(0,l)}+\|\bar{v}_x(t)\|_{L^2(0,l)}\\ &\quad+\|\gamma\bar{w}(t)-\alpha\bar{\phi}(t)\|_{L^2(0,l)})\\ &\leq\; c[(c_G+c_p|\gamma|)\|\bar{w}(t)\|_{H^1(0,l)}+\|\bar{v}(t)\|_{H^1(0,l)}\\ &\quad+(|\gamma|+c_p|\alpha|)\|\bar{\phi}_x(t)\|_{H^1(0,l)}]\\ &\leq\; L\|\bar{\mathbf{u}}(t)\|_{H^1}\\ &\leq\; L(\|\bar{\mathbf{u}}(t)-\mathbf{u}_0\|_{H^1}+\|\mathbf{u}_0\|_{H^1}).\end{aligned}$$

Applying the bound in (3.28),

$$\|\mathbf{f}(\bar{\mathbf{u}}(t))\|_{L^2} \leq L(r + \|\mathbf{u}_0\|_{H^1}) < \infty.$$

Thus,

$$\int_0^{t_1} \|f(\bar{\mathbf{u}}(t))\|_{L^2} dt \leq \int_0^{t_1} L(r + \|\mathbf{u}_0\|_{H^1}) dt < \infty.$$

Thus, by Theorem 3.22, $\bar{\mathbf{u}}$ is a strong solution of the initial value problem (3.22) and (3.23).

We now define the function $\mathbf{F}(t, \mathbf{u}(t)) := \mathbf{u}_t(t) - \mathbf{f}(t, \mathbf{u}(t))$. The solution, $\bar{\mathbf{u}}$, of the initial value problem (3.22) and (3.23) is also a solution of

$$\begin{aligned} \mathbf{A}\mathbf{u}(t) &= \mathbf{F}(t, \mathbf{u}(t)) \\ \mathbf{u}(0) &= \mathbf{u}_0. \end{aligned}$$

By the definition of a strong solution, $t \to \mathbf{f}(t, \bar{\mathbf{u}}(t))$ is locally Hölder continuous on $L^2(0,l)^3$ for $t \in (0, t_1)$. Likewise, by Theorem 3.24, since $\mathbf{A}$ is sectorial, $(0, u_0) \in N_\delta(0, \mathbf{u}_0)$ and $\mathbf{f} : N_\delta(0, \mathbf{u}_0) \to L^2(0,l)^3$ is locally Lipschitz, $t \to \bar{\mathbf{u}}_t(t)$ is locally Hölder continuous on $H_0^1(0,l)^3$ for $t \in (0, t_1)$. Since Hölder continuity is stronger than continuity, $t \to \mathbf{F}(t, \bar{\mathbf{u}}(t))$ is locally continuous on $L^2(0,l)^3$ for $t \in (0, t_1)$. Thus, by elliptic regularity,

$$\begin{aligned} \bar{\mathbf{u}} \in\ & C([0,t_1); (H_0^1(0,l)^3) \cap C^1([0,t_1); (H_0^1(0,l)^3) \cap \\ & \quad C((0,t_1); (H^2(0,l) \cap H_0^1(0,l))^3) \\ & \subset C^1([0,t_1); (H_0^1(0,l)^3) \cap C((0,t_1); (H^2(0,l) \cap H_0^1(0,l)^3) \end{aligned}$$

Therefore, $\bar{\mathbf{u}}$ is a classical solution which, in turn, implies that

$$\begin{aligned} \bar{w} &\in C([0,t_1); H_0^1(0,l)) \cap C^1((0,t_1); H_0^1(0,l)) \cap C((0,t_1); H^2(0,l)) \\ \bar{v} &\in C([0,t_1); H_0^1(0,l)) \cap C^1((0,t_1); H_0^1(0,l)) \cap C((0,t_1); H^2(0,l)) \\ \bar{\phi} &\in C([0,t_1); H_0^1(0,l)) \cap C^1((0,t_1); H_0^1(0,l)) \cap C((0,t_1); H^2(0,l)). \end{aligned}$$

The proof of Theorem 3.1 is complete.

Chapter 4

Numerical Analysis for the Temperature Independent Model

4.1 Introduction

In this chapter we begin by reviewing a finite element method for a parabolic partial differential equation. We then expand this discussion to a system of parabolic equations and present error estimates for the semidiscrete scheme, closely following Wheeler [95]. Finally, we derive an fully discretized algorithm for solving the temperature independent system (2.44)-(2.52) using a Crank-Nicolson-Galerkin finite element scheme.

4.2 A review of the finite element method

In this section we review some basic ideas behind the finite element method for a parabolic partial differential equation in one space dimension. For the discussion on interpolation we follow Ciarlet [42]. For the discussion on discretization of parabolic differential equations we follow Thomée [93].

In this discussion we consider the following boundary value problem:

$$u_t(x,t) = u_{xx}(x,t) + f(x,t) \qquad (x,t) \in [a,b] \times (0,T] \tag{4.1}$$

$$u(a,t) = u(b,t) = 0 \quad t \in (0,T] \tag{4.2}$$

$$u(x,0) = u_0(x) \quad x \in [a,b] \tag{4.3}$$

where $f : [a,b] \times (0,T] \to \mathbb{R}$ is Lipschitz continuous in both arguments. We will also assume that there exists a unique solution, u, to the above initial value problem such that $u \in C([0,T]; H^2(a,b) \cap H_0^1(a,b)) \cap C^1((0,T); L^2(a,b))$.

Our strategy is such that, for each fixed t, we will approximate the solution, $u(x,t)$, to the above initial value problem by a function $u_h(x,t) \in S_h$, where $S_h \subset H^1(a,b)$ is a finite dimensional space of functions with certain approximation properties. The semidiscrete solution, u_h, will be the solution of a system of ordinary differential equations in t. We will then discretize the resulting system of differential equations in t to obtain a fully discrete scheme to approximate u.

4.2.1 Interpolation

To begin, we create a partition of $[a, b]$. Let N be a positive integer. We define a partition $\Delta_{[a,b]}$ by

$$\Delta_{[a,b]} = \{a = x_0 < x_1 < \cdots < x_i < \cdots < x_{N-1} < x_N = b\}$$

where $x_i = a + ih, i = 0, 1, \cdots N$, and $h = \dfrac{(b-a)}{N}$. A function on $[a, b]$ is said to be piecewise linear if it is linear on each interval $[x_i, x_{i+1}], i = 0, 1, \cdots, N-1$. Let $P_1[a, b]$ denote the set of continuous piecewise linear functions on $[a, b]$. We define the space S^h to be

$$S_h = \{\psi(x) : \psi \in P_1[a, b], \psi(a) = \psi(b) = 0\}. \tag{4.4}$$

We now define the following "hat" functions in S_h. For $1 \leq j \leq N-1$, define $\psi_j \in S_h$ by

$$\psi_j(x) = \begin{cases} \dfrac{x - x_{j-1}}{h} & x_{j-1} \leq x \leq x_j \\ \dfrac{x_{j+1} - x}{h} & x_j \leq x \leq x_{j+1} \\ 0 & elsewhere. \end{cases} \tag{4.5}$$

We note that

$$\psi_j(x_i) = \delta_{ij} = \begin{cases} 1 & i = j \\ 0 & i \neq j \end{cases}$$

for $1 \leq j \leq N-1, 0 \leq i \leq N$. The space S_h is an $N-1$ dimensional subspace of $H_0^1(a, b)$. The functions $\{\psi_j\}_{j=1}^{N-1}$ form a basis for S_h.

We will use functions in S_h to approximate the solution to (4.1)-(4.3). Thus, we need to establish some approximation properties of S_h.

Proposition 4.1 *Let $v \in C_0[a, b]$, the space of continuous functions on (a, b) with compact support. There is a unique $v_h \in S_h$ such that $v(x_i) = v_h(x_i)$ for $1 \leq i \leq N-1$.*

Proof. Define v_h by

$$v_h(x) = \sum_{j=1}^{N-1} v(x_j)\psi_j(x).$$

then $v_h \in S_h$ and $v(x_i) = v_h(x_i)$ for $0 \leq i \leq N$. Uniqueness follows from the fact that if there were two such functions v_h^1 and $v_h^2 \in S_h$, then $(v_h^1 - v_h^2)(x_i) = 0$ for $0 \leq i \leq N$. Since $v_h^1 - v_h^2$ is piecewise linear and continuous, then $v_h^1 - v_h^2$ is identically zero on $[a, b]$. ■

We call v_h the S_h interpolant of v and denote v_h by $I_h v$. For any $v \in C_0[a,b]$, we may write $I_h v$ as the following

$$I_h v(x) = \sum_{j=1}^{N-1} v(x_j)\psi_j(x).$$

The following result gives important error estimates for the S_h interpolant of v.

Theorem 4.2 *Let $v \in H_0^1(a,b)$ and suppose $I_h v$ is the S_h interpolant of v. Then there exists constants C_1, C_2, C_3, independent of h and v, such that*

$$\|v - I_h v\|_{L^2(a,b)} \leq C_1 h \|v\|_{H_0^1(a,b)}.$$

If, in addition, $v \in H^2(a,b) \cap H_0^1(a,b)$ then

$$\begin{aligned} \|v - I_h v\|_{L^2(a,b)} &\leq C_2 h^2 \|v\|_{H^2(a,b)} && (4.6) \\ \|v - I_h v\|_{H_0^1(a,b)} &\leq C_3 h \|v\|_{H^2(a,b)}. && (4.7) \end{aligned}$$

For a more general version of Theorem 4.2 see Ciarlet [42, p. 139].

Define the bilinear form $B : H_0^1(a,b) \times H_0^1(a,b)$ by

$$B(u,v) := \langle u_x, v_x \rangle_{L^2(a,b)}.$$

Lemma 4.3 *Let $u \in H_0^1(a,b)$. There is a unique $w_h \in S_h$ such that*

$$B(w_h, \psi) = B(u, \psi) \tag{4.8}$$

for all $\psi \in S_h$. Moreover, there exists a constant C such that

$$\|u - w_h\|_{H_0^1(a,b)} \leq C \inf_{\psi \in S_h} \|u - \psi\|_{H_0^1(a,b)}.$$

The function w_h is called the elliptic projection of u into S_h. A more general version of Proposition 4.3 may be found in Ciarlet [42, pp. 104-5]. The following lemma relates the elliptic projection to the S_h interpolant.

Lemma 4.4 *The solution w_h of (4.8) is the S_h interpolant of $v \in H_0^1(a,b)$, that is,*

$$w_h(x_i) = v(x_i)$$

for $1 \leq i \leq N$.

See Ciarlet [42, p. 105].

In the case where one or more of the boundary conditions (4.2) are nonzero or include a derivative, we define our interpolation space differently. For example, suppose the boundary conditions are

$$u(a,t) = \alpha, \quad u_x(b,t) = \beta \quad t \in [0,T]. \tag{4.9}$$

We modify our approach by defining the following interpolation space

$$\tilde{S}_h = \{\psi(x) : \psi \in P_1[a,b]\} \tag{4.10}$$

with respect to the partition $\Delta_{[a,b]}$. The set $\tilde{S}_h$ is an $N+1$ dimensional subspace of $H^1(a,b)$. The basis of hat functions for $\tilde{S}_h$ is given by $\{\tilde{\psi}_j(x)\}_{j=0}^{N}$. Here $\tilde{\psi}_j(x) = \psi_j(x), 1 \le j \le N-1$ where ψ_j is defined by (4.5) and

$$\psi_0(x) = \begin{cases} \dfrac{x_0 - x}{h} & a \le x \le x_1 \\ 0 & elsewhere \end{cases} \tag{4.11}$$

and

$$\psi_N(x) = \begin{cases} \dfrac{x - x_{N-1}}{h} & x_{N-1} \le x \le b \\ 0 & elsewhere. \end{cases} \tag{4.12}$$

We define the interpolant in $\tilde{S}_h$, $\tilde{I}_h v$, to be a continuous function $v \in H^1(a,b)$ by $(\tilde{I}_h v)(x_i) = v(x_i), 0 \le i \le N$. The $\tilde{S}_h$ interpolant is unique and for any $v \in C[a,b]$ satisfying the boundary conditions (4.9), we may write $I_h v$ as the following

$$\tilde{I}_h v(x) = \alpha\psi_0(x) + \sum_{j=1}^{N} v(x_j)\psi_j(x).$$

Similar error estimates exist for the $\tilde{S}_h$ interpolant see Ciarlet [42].

4.2.2 Discretization techniques

Any solution of the initial boundary value problem (4.1)-(4.3) is also a solution of

$$\langle u_t, v\rangle_{L^2(a,b)} = -\langle u_x, v_x\rangle_{L^2(a,b)} + \langle f, v\rangle_{L^2(a,b)}, \quad t > 0$$

for all $v \in H_0^1[a,b]$. It is this weak formulation of (4.1)-(4.3) that we use in the finite element method. For any fixed $t > 0$, we define the finite element solution of the initial boundary value problem (4.1)-(4.3) to be the function $u_h(t) \in S_h$ which satisfies

$$\langle u_{h,t}, \psi\rangle_{L^2(a,b)} = -\langle u_{h,x}, \psi_x\rangle_{L^2(a,b)} + \langle f, \psi\rangle_{L^2(a,b)}, \quad t > 0 \tag{4.13}$$

for all $\psi \in S_h$ along with the initial condition $u_h(0) = v_h$ where v_h is some approximation of u_0 in S_h. We call equation (4.13) the semidiscrete problem. Using the basis functions of S_h, we may write u_h as

$$u_h(x,t) = \sum_{j=1}^{N-1} a_j(t)\psi_j(x).$$

Thus the semidiscrete problem may be posed in terms of the basis $\{\psi_j\}_{j=1}^{N-1}$ as:
Find the coefficient functions, $a_j(t), 1 \leq j \leq N-1$, such that

$$\sum_{j=1}^{N-1} a_j'(t)\langle \psi_j, \psi_i\rangle_{L^2(a,b)} = -\sum_{j=1}^{N-1} a_j(t)\langle \psi_{j,x}, \psi_{i,x}\rangle_{L^2(a,b)} + \langle f, \psi_i\rangle_{L^2(a,b)}, \quad t > 0$$

for $1 \leq i \leq N-1$. In matrix notation, the above system may be written as

$$M\mathbf{a}'(t) + S\mathbf{a}(t) = \mathbf{f}(t), \quad t > 0 \tag{4.14}$$

with $\mathbf{a}(0) = [v_h(x_1), \cdots, v_h(x_{N-1})]^T, M = [M_{i,j}] = [\langle \psi_j, \psi_i\rangle_{L^2(a,b)}]$,
$S = [S_{i,j}] = [\langle \psi_{j,x}, \psi_{i,x}\rangle_{L^2(a,b)}]$ and $\mathbf{f} = [\mathbf{f}_i] = [\langle f, \psi_i\rangle_{L^2(a,b)}], 1 \leq i,j \leq N-1$. The matrices, M and S, are referred to as the mass and stiffness matrices, respectively. Since the mass matrix, M, is positive definite and invertible and $\tilde{\mathbf{f}}$ is Lipschitz continuous in t, the differential system (4.14) has a unique solution, u_h, which is a continuous function of t.

The following result gives an estimate for the error between the semidiscrete solution and the exact solution.

Theorem 4.5 *Let u and u_h be the solutions of (4.1) and (4.13), respectively. Then*

$$\|u_h(t) - u(t)\|_{L^2(a,b)} \leq \|v_h - u_0\|_{L^2(a,b)} + Ch^2\{\|u_0\|_{H^2(a,b)} + \int_0^t \|u_t\|_{H^2(a,b)} ds\} \quad t > 0.$$

For a proof of Theorem 4.5 see Thomée [96, pp. 5-8].

There are several methods for solving the semidiscrete problem (4.14), see Thomée [93]. One such method is the Crank-Nicolson-Galerkin method in which the semidiscrete problem is discretized about the point $t_{n-\frac{1}{2}}$.

Let τ be the time step. We define $u_h^n \in S_h$ recursively by

$$\langle \frac{u_h^n - u_h^{n-1}}{\tau}, \psi\rangle_{L^2(a,b)} + \langle \frac{u_{h,x}^n + u_{h,x}^{n-1}}{2}, \psi_x\rangle_{L^2(a,b)} = \langle f(t_{n-\frac{1}{2}}), \psi\rangle_{L^2(a,b)} \tag{4.15}$$

for all $\psi \in S_h$ and $u_h^0 = v_h$. The matrix equation for (4.15) is

$$(M + \frac{1}{2}\tau S)\mathbf{a}^n = (M - \frac{1}{2}\tau S)\mathbf{a}^{n-1} + \tau\tilde{f}(t_{n-\frac{1}{2}})$$

with the matrix $(M + \frac{1}{2}\tau S)$ positive definite and invertible. Assuming enough smoothness on u yields the following error estimate.

Theorem 4.6 *Let u and u_h^n be the solutions of (4.1) and (4.15) respectively. If u is such that u_t and u_x are twice continuously differentiable in t on $(0,T)$ and $u_{ttt}, u_{xtt} \in L^2(a,b)$ for $t \in (0,T)$, then, for $t > 0$,*

$$\begin{aligned} \|u_h^n - u(t_n)\|_{L^2(a,b)} \;\; &\leq \;\; \|v_h - u_0\|_{L^2(a,b)} + Ch^2\{\|u_0\|_{H^2(a,b)} + \int_0^{t_n} \|u_t\|_{H^2(a,b)} ds\} \\ &\quad + C\tau^2 \int_0^{t_n} (\|u_{ttt}\|_{L^2(a,b)} + \|u_{xtt}\|_{L^2(a,b)}) ds. \end{aligned} \tag{4.16}$$

A proof of Theorem 4.6 may be found in Thomée [96, pp. 14-15].

4.3 Finite element method for systems of nonlinear parabolic partial differential equations

In this section we extend the finite element method discussed in Section 4.2 to systems of nonlinear equations with homogeneous boundary conditions. Let Ω be a bounded subset of $\mathbb{R}$. We consider the following initial value problem with homogeneous boundary conditions: Let $\mathbf{u}(x,t) = \begin{bmatrix} u_1(x,t) \\ u_2(x,t) \\ u_3(x,t) \end{bmatrix}$. We wish to solve

$$\begin{bmatrix} u_{1t} \\ u_{2t} \\ u_{3t} \end{bmatrix} = \begin{bmatrix} \alpha_1 u_{1,xx} \\ \alpha_2 u_{2,xx} \\ \alpha_3 u_{3,xx} \end{bmatrix} + \begin{bmatrix} f_1(\mathbf{u}, \mathbf{u}_x) \\ f_2(\mathbf{u}, \mathbf{u}_x) \\ f_3(\mathbf{u}, \mathbf{u}_x) \end{bmatrix}, \quad (x,t) \in \Omega \times (0,T) \tag{4.17}$$

$$\mathbf{u}(x,t) = \mathbf{0} \quad (x,t) \in \partial\Omega \times (0,T) \tag{4.18}$$

$$\mathbf{u}(x,0) = \mathbf{u}_0(x) \quad x \in \Omega. \tag{4.19}$$

We introduce some notation needed in the subsequent discussion.

Definition 4.7 *Let H be a Hilbert space defined on Ω. If w is a function defined on $[0,T] \times \Omega$, we say $w \in L^p([0,T];H), 1 \leq p \leq \infty$, if for $t \in [0,T]$, we have $w(\cdot,t) \in H$ and $\|w\|_H \in L^p([0,T])$. We define*

$$\|w\|_{L^p([0,t];H)} = \|F(t)\|_{L^p([0,t])}$$

where $F(t) = \|w(\cdot,t)\|_H$.

We define the bilinear form $\mathbf{B}(\cdot,\cdot) : H_0^1(\Omega)^3 \times H_0^1(\Omega)^3 \to \mathrm{I\!R}$ by

$$\mathbf{B}(\mathbf{u},\mathbf{v}) = \langle \alpha_1 u_{1,x}, v_{1,x}\rangle + \langle \alpha_2 u_{2,x}, v_{2,x}\rangle + \langle \alpha_3 u_{3,x}, v_{3,x}\rangle.$$

We know that if $\mathbf{u}$ is a solution of (4.17) then $\mathbf{u}$ satisfies

$$\left\langle \begin{bmatrix} u_{1,t} \\ u_{2,t} \\ u_{3,t} \end{bmatrix}, \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \right\rangle = -\mathbf{B}(\mathbf{u},\mathbf{v}) + \left\langle \begin{bmatrix} f_1(\mathbf{u},\mathbf{u}_x) \\ f_2(\mathbf{u},\mathbf{u}_x) \\ f_3(\mathbf{u},\mathbf{u}_x) \end{bmatrix}, \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \right\rangle \tag{4.20}$$

$$\left\langle \begin{bmatrix} u_1(x,0) \\ u_2(x,0) \\ u_3(x,0) \end{bmatrix}, \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \right\rangle = \left\langle \begin{bmatrix} u_{1,0} \\ u_{2,0} \\ u_{3,0} \end{bmatrix}, \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \right\rangle$$

for all $\mathbf{v} \in H_0^1(\Omega)^3$. A function, $\mathbf{u} = \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix} \in C^1([0,T]; H_0^1(\Omega)^3)$, which satisfies (4.20) is said to be a weak solution of (4.17).

Without loss of generality we set $\Omega = [a,b]$. Define the partition $\Delta_\Omega = \{a = x_0 < x_1 < \cdots x_i < \cdots < x_{N-1} < x_N = b\}$ where $x_i = a + ih, 0 \le i \le N$ and $h = \dfrac{b-a}{N}$. We define the finite element space $\mathbf{S}_h$ by

$$\mathbf{S}_h = \left\{ \begin{bmatrix} y_1(x) \\ y_2(x) \\ y_3(x) \end{bmatrix} : y_i \in S_h, i = 1,2,3 \right\}$$

where S_h is the finite element space defined by (4.4).

Let $\{\psi_j^i\}_{j=1}^{N-1}$ be the basis of hat functions for S_h defined by (4.4), for each $i = 1,2,3$. As an approximation to $\mathbf{u}$ at some fixed time, t, we seek a function

$$\mathbf{U}(x,t) = \begin{bmatrix} \sum_{j=1}^{N-1} a_j(t)\psi_j^1(x) \\ \sum_{j=1}^{N-1} b_j(t)\psi_j^2(x) \\ \sum_{j=1}^{N-1} c_j(t)\psi_j^3(x) \end{bmatrix}, \in \mathbf{S}_h \tag{4.21}$$

such that

$$\left\langle \begin{bmatrix} U_{1,t} \\ U_{2,t} \\ U_{3,t} \end{bmatrix}, \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right\rangle = -\mathbf{B}(\mathbf{U},\mathbf{y}) + \left\langle \begin{bmatrix} f_1(\mathbf{U},\mathbf{U}_x) \\ f_2(\mathbf{U},\mathbf{U}_x) \\ f_3(\mathbf{U},\mathbf{U}_x) \end{bmatrix}, \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right\rangle \tag{4.22}$$

$$\begin{bmatrix} U_1(x,0) \\ U_2(x,0) \\ U_3(x,0) \end{bmatrix} = \begin{bmatrix} U_{1,0}(x) \\ U_{2,0}(x) \\ U_{3,0}(x) \end{bmatrix} \tag{4.23}$$

for all $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \in \mathbf{S}_h$ where $\begin{bmatrix} U_{1,0}(x) \\ U_{2,0}(x) \\ U_{3,0}(x) \end{bmatrix}$ is an approximation in $\mathbf{S}_h$ of $\mathbf{u}_0 = \begin{bmatrix} u_{1,0} \\ u_{2,0} \\ u_{3,0} \end{bmatrix}$.
We refer to (4.22) as the semidiscrete finite element problem and $\mathbf{U}$ as the finite element solution.

Define $\mathbf{a}(t) = [a_j(t)]_{j=1}^{N-1}$, $\mathbf{b}(t) = [b_j(t)]_{j=1}^{N-1}$ and $\mathbf{c}(t) = [c_j(t)]_{j=1}^{N-1}$. Then the equations (4.22) and (4.23) can be reduced to an initial value problem for the system of nonlinear ordinary differential equations in t of the form

$$\mathbf{A}\begin{bmatrix} \mathbf{a}'(t) \\ \mathbf{b}'(t) \\ \mathbf{c}'(t) \end{bmatrix} = \mathbf{D}\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix} + \mathbf{F}\left(\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix}\right) \tag{4.24}$$

$$\begin{bmatrix} \mathbf{a}(0) \\ \mathbf{b}(0) \\ \mathbf{c}(0) \end{bmatrix} = \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{bmatrix}. \tag{4.25}$$

Here $\mathbf{A} = \begin{bmatrix} M & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & M & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & M \end{bmatrix}$, $\mathbf{D} = \begin{bmatrix} S & \mathbf{0} & \mathbf{0} \\ \mathbf{0} & S & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & S \end{bmatrix}$ where M and S are the mass and stiffness matrices of dimension $N-1 \times N-1$. The function $\mathbf{F}$ is given by

$$\mathbf{F}\left(\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix}\right) = \begin{bmatrix} \langle f_1(\mathbf{U}, \mathbf{U}_x), \psi_1^1 \rangle \\ \vdots \\ \langle f_1(\mathbf{U}, \mathbf{U}_x), \psi_{N-1}^1 \rangle \\ \langle f_2(\mathbf{U}, \mathbf{U}_x), \psi_1^2 \rangle \\ \vdots \\ \langle f_2(\mathbf{U}, \mathbf{U}_x), \psi_{N-1}^2 \rangle \\ \langle f_3(\mathbf{U}, \mathbf{U}_x), \psi_1^3 \rangle \\ \vdots \\ \langle f_3(\mathbf{U}, \mathbf{U}_x), \psi_{N-1}^3 \rangle \end{bmatrix}$$

where $\mathbf{U}$ as a function of $\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix}$ is given by (4.21) and $\mathbf{U}_x$ is given by

$$\mathbf{U}_x(x,t) = \begin{bmatrix} \sum_{j=1}^{N-1} a_j(t)\psi_{j,x}^1(x) \\ \sum_{j=1}^{N-1} b_j(t)\psi_{j,x}^2(x) \\ \sum_{j=1}^{N-1} c_j(t)\psi_{j,x}^3(x) \end{bmatrix}.$$

In order to continue, we need the following lemma.

Lemma 4.8 *Let $r > 0$ be as in Theorem 3.21. Let*

$$D_r = \left\{ \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \\ \mathbf{z} \end{bmatrix} \in \mathbb{R}^{3N-3} : \left\| \begin{bmatrix} \mathbf{x} \\ \mathbf{y} \\ \mathbf{z} \end{bmatrix} - \begin{bmatrix} \mathbf{a}_0 \\ \mathbf{b}_0 \\ \mathbf{c}_0 \end{bmatrix} \right\|_{l^2} < r \right\}$$

Suppose $\mathbf{F}$ is locally Lipschitz on $\mathbb{R}^{3N-3} \times \mathbb{R}^{3N-3}$. Then there exists $T_1 > 0$ and $r > 0$ such the initial value problem (4.24) and (4.25) has a unique solution, $\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix} \in C^1(0,T)$, with $\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix} \in D_r, 0 \le t \le T_1$.

This existence result may be found in any standard ODE text (see [43] for example). It uses the fact that $\mathbf{F}$ is locally Lipschitz in $\begin{bmatrix} \mathbf{a}(t) \\ \mathbf{b}(t) \\ \mathbf{c}(t) \end{bmatrix}$. Then, since $\mathbf{A}$ is invertible, the initial value problem (4.24) and (4.25) has a unique solution on some bounded neighborhood of $\mathbf{U}_0$. This implies that there exists $M^* > 0$ such that $\|\mathbf{U}\|_{L^\infty(\Omega)}, \|\mathbf{U}_x\|_{L^\infty(\Omega)} < M^*$ on $[0, T_1]$.

For any $\mathbf{u} \in H_0^1(\Omega)^3$, we define $\tilde{\mathbf{u}} \in \mathbf{S}_h$ by

$$\mathbf{B}((\mathbf{u} - \tilde{\mathbf{u}}), \mathbf{v}) = 0, \tag{4.26}$$

for all $\mathbf{v} \in \mathbf{S}_h$, here

$$\tilde{u}_i(x,t) = \begin{bmatrix} \sum_{j=1}^{N-1} \tilde{a}_j(t)\psi_j^1(x) \\ \sum_{j=1}^{N-1} \tilde{b}_j(t)\psi_j^2(x) \\ \sum_{j=1}^{N-1} \tilde{c}_j(t)\psi_j^3(x) \end{bmatrix}$$

where the set $\left\{ \begin{bmatrix} \psi_j^1 \\ \psi_j^2 \\ \psi_j^3 \end{bmatrix} \right\}_{j=1}^{M}$ form a basis for $\mathbf{S}_h$. We say $\tilde{\mathbf{u}}$ is the elliptic projection of $\mathbf{u}$ into $\mathbf{S}_h$.

We now present error estimates for the finite element solution $\mathbf{U}$. We choose $\mathbf{u}_0 \in H_0^1(\Omega)^3$ and $r > 0$. Then by Theorem 3.21, there exists $T_2 > 0$ such that there exists a unique solution, $\mathbf{u} \in C((0,T_2); H_0^1(\Omega)^3)$ to the initial value problem (4.17) with $\|\mathbf{u} -$

$\mathbf{u}_0\|_{H_0^1(\Omega)^3} < r$ on $[0, T_2]$. Thus there exists $\hat{M} > 0$ such that $\|\mathbf{u}\|_{L^\infty(\Omega)}, \|\mathbf{u}_x\|_{L^\infty(\Omega)} < \hat{M}$ on $[0, T_2]$. From Lemma 4.8 we know there exists $T_1 > 0$ such that the finite element solution, $\mathbf{U}$ satisfies $\|\mathbf{U} - \mathbf{U}_0\|_{L^\infty} < r$ on $[0, T_1]$.

Let $\bar{T} = \min\{T_1, T_2\}$. Let $\tilde{M} = \max\{r, M^*, \hat{M}\}$. Let $D = [-\tilde{M}, \tilde{M}]^3$. We assume the following about the initial value problem (4.17)-(4.19).

Hypothesis 4.9 • *The bilinear form,* $\mathbf{B}$ *satisfies*

$$0 < \nu_1 \|\mathbf{u}\|^2_{H_0^1(\Omega)^3} \leq \mathbf{B}(\mathbf{u}, \mathbf{u}) \leq \nu_2 \|\mathbf{u}\|^2_{H_0^1(\Omega)^3} < \infty \tag{4.27}$$

where $\nu_1 = \min\{\alpha_1, \alpha_2, \alpha_3\}$ *and* $\nu_2 = \max\{\alpha_1, \alpha_2, \alpha_3\}$.

- $\mathbf{u}_0 \in [H^2(\Omega) \cap H_0^1(\Omega)]^3$.

- $\mathbf{u} \in C((0, \bar{T}); (H^2(0, l) \cap H_0^1(0, l)^3) \cap C^1([0, \bar{T}); (H_0^1(0, l)^3)$ *is the unique solution of the initial value problem (4.17), with* $\mathbf{u} \in L^2([0, \bar{T}]; [H^2(\Omega) \cap H_0^1(\Omega)]^3)$,
  $\mathbf{u}_t \in L^2([0, \bar{T}]; [H_0^1(\Omega)^3)$ *and* $\|\mathbf{u} - \mathbf{u}_0\|_{H_0^1(\Omega)^3} < r$ *for* $t \in [0, \bar{T}]$.

- *Let* $|\cdot|$ *denote absolute value in* $\mathbb{R}$ *and* $|\cdot|_{l^2}$ *denote the* l^2 *norm on* $\mathbb{R}^3$. *The functions* $f_i(\cdot, \cdot) : D \times D \to \mathbb{R}$ *are Lipschitz in both arguments, for* $i = 1, 2, 3$, *that is, there exists* $L > 0$ *such that for* $\mathbf{x}_1, \mathbf{x}_2, \mathbf{y}_1, \mathbf{y}_2 \in D$,

$$\begin{aligned} |f_i(\mathbf{x}_1, \mathbf{y}) - f_i(\mathbf{x}_2, \mathbf{y})| &\leq L|\mathbf{x}_1 - \mathbf{x}_2|_{l^2} \\ |f_i(\mathbf{x}, \mathbf{y}_1) - f_i(\mathbf{x}, \mathbf{y}_2)| &\leq L|\mathbf{y}_1 - \mathbf{y}_2|_{l^2}. \end{aligned}$$

Theorem 4.10 *Let* $D, \tilde{M}$ *and* $\bar{T}$ *be as described above. Suppose Hypothesis 4.9 holds. Let* $\mathbf{U} = [U_1, U_2, U_3]^T$ *be the solution of the finite element problem (4.22) and (4.23). Then, for* $\tau \in [0, \bar{T}]$, *there exists* $\delta \geq 0$ *such that*

$$\begin{aligned} \|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) \quad + \quad & \delta \|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2((0,\tau), H_0^1(\Omega)^3)} \leq C_1^* \|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(0) \\ & + C_2^* \|(\mathbf{u} - \tilde{\mathbf{u}})_t\|^2_{L^2((0,\tau), L^2(\Omega)^3)} + C_3^* \|\tilde{\mathbf{u}} - \mathbf{u}\|^2_{L^2((0,\tau), H_0^1(\Omega)^3)} \end{aligned}$$

where $C_1^*, C_2^*, C_3^* > 0$ *depend only on* τ, ν_1 *and* L.

Proof. Let $\mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \in \mathbf{S}^h$. Using (4.26) and (4.20) we have

$$\left\langle \begin{bmatrix} \tilde{u}_{1,t} \\ \tilde{u}_{2,t} \\ \tilde{u}_{3,t} \end{bmatrix}, \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right\rangle = -\mathbf{B}(\tilde{\mathbf{u}}, \mathbf{y}) + \left\langle \begin{bmatrix} (\tilde{u}_1 - u_1)_t \\ (\tilde{u}_2 - u_2)_t \\ (\tilde{u}_3 - u_3)_t \end{bmatrix}, \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right\rangle + \left\langle \begin{bmatrix} f_1(\mathbf{u}, \mathbf{u}_x) \\ f_2(\mathbf{u}, \mathbf{u}_x) \\ f_3(\mathbf{u}, \mathbf{u}_x) \end{bmatrix}, \begin{bmatrix} y_1 \\ y_2 \\ y_3 \end{bmatrix} \right\rangle. \tag{4.28}$$

We note that for $\mathbf{u}, \mathbf{v} \in L^2(\Omega)^3$,

$$\langle \mathbf{u}, \mathbf{v} \rangle = \left\langle \begin{bmatrix} u_1 \\ u_2 \\ u_3 \end{bmatrix}, \begin{bmatrix} v_1 \\ v_2 \\ v_3 \end{bmatrix} \right\rangle = \sum_{i=1}^{3} \langle u_i, v_i \rangle. \tag{4.29}$$

Subtracting (4.28) from (4.22) and setting $\mathbf{y} = \mathbf{U} - \tilde{\mathbf{u}}$, we have

$$\begin{aligned} \langle (\mathbf{U} - \tilde{\mathbf{u}})_t, \mathbf{U} - \tilde{\mathbf{u}} \rangle &= \sum_{i=1}^{3} \langle (U_i - \tilde{u}_i)_t, U_i - \tilde{u}_i \rangle \\ &= -\mathbf{B}(\mathbf{U} - \tilde{\mathbf{u}}, \mathbf{U} - \tilde{\mathbf{u}}) + \sum_{i=1}^{3} \{ \langle (u_i - \tilde{u}_i)_t, U_i - \tilde{u}_i \rangle \\ &\quad + \langle (f_i(\mathbf{U}, \mathbf{U}_x) - f_i(\mathbf{u}, \mathbf{u}_x)), U_i - \tilde{u}_i \rangle \}. \end{aligned}$$

Thus

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} (\|\mathbf{U} - \tilde{\mathbf{u}}\|_{L^2}^2) &\leq -\mathbf{B}(\mathbf{U} - \tilde{\mathbf{u}}, \mathbf{U} - \tilde{\mathbf{u}}) + \sum_{i=1}^{3} \{ \langle |(u_i - \tilde{u}_i)_t|, |U_i - \tilde{u}_i| \rangle \\ &\quad + \langle |f_i(\mathbf{U}, \mathbf{U}_x) - f_i(\mathbf{u}, \mathbf{u}_x)|, |U_i - \tilde{u}_i| \rangle \}. \end{aligned}$$

Now, we know

$$\begin{aligned} |f_i(\mathbf{U}, \mathbf{U}_x) - f_i(\mathbf{u}, \mathbf{u}_x)| &\leq |f_i(\mathbf{U}, \mathbf{U}_x) - f_i(\mathbf{U}, \mathbf{u}_x)| + |f_i(\mathbf{U}, \mathbf{u}_x) - f_i(\mathbf{u}, \mathbf{u}_x)| \\ &\leq L(|\mathbf{U}_x - \mathbf{u}_x|_{l^2} + |\mathbf{U} - \mathbf{u}|_{l^2}). \end{aligned}$$

Thus we have, using (4.27),

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} (\|\mathbf{U} - \tilde{\mathbf{u}}\|_{L^2(\Omega)^3}^2) &\leq -\nu_1 \|\mathbf{U} - \tilde{\mathbf{u}}\|_{H_0^1(\Omega)^3}^2 + \sum_{i=1}^{3} \{ \langle |(u_i - \tilde{u}_i)_t|, |U_i - \tilde{u}_i| \rangle \\ &\quad + L \langle (|\mathbf{U}_x - \mathbf{u}_x)|_{l^2} + |\mathbf{U} - \mathbf{u}|_{l^2}), |U_i - \tilde{u}_i| \rangle \}. \end{aligned}$$

Applying Hölder's inequality , we have

$$\begin{aligned} \frac{1}{2} \frac{d}{dt} (\|\mathbf{U} - \tilde{\mathbf{u}}\|_{L^2(\Omega)^3}^2) &\leq -\nu_1 \|\mathbf{U} - \tilde{\mathbf{u}}\|_{H_0^1(\Omega)^3}^2 + \sum_{i=1}^{3} \|(u_i - \tilde{u}_i)_t\|_{L^2(\Omega)} \|U_i - \tilde{u}_i\|_{L^2(\Omega)} \\ &\quad + L \sum_{i=1}^{3} \sum_{j=1}^{3} \|U_j - u_j\|_{H_0^1(\Omega)} \|U_i - \tilde{u}_i\|_{L^2(\Omega)} \\ &\quad + L \sum_{i=1}^{3} \sum_{j=1}^{3} \|U_j - u_j\|_{L^2(\Omega)} \|U_i - \tilde{u}_i\|_{L^2(\Omega)}. \end{aligned}$$

Applying the triangle inequality, we have

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}(\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}) \;\; \le \;\; & -\nu_1\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{H^1_0(\Omega)^3}+\sum_{i=1}^{3}\|(u_i-\tilde{u}_i)_t\|_{L^2(\Omega)}\|U_i-\tilde{u}_i\|_{L^2(\Omega)}\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}\|U_j-\tilde{u}_j\|_{H^1_0(\Omega)}\|U_i-\tilde{u}_i\|_{L^2(\Omega)}\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}\|\tilde{u}_j-u_j\|_{H^1_0(\Omega)}\|U_i-\tilde{u}_i\|_{L^2(\Omega)}\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}\|U_j-\tilde{u}_j\|_{L^2(\Omega)}\|U_i-\tilde{u}_i\|_{L^2(\Omega)}\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}\|\tilde{u}_j-u_j\|_{L^2(\Omega)}\|U_i-\tilde{u}_i\|_{L^2(\Omega)}.\end{aligned}$$

Now use the inequality $ab \le \frac{1}{2}(\epsilon a^2+\frac{1}{\epsilon}b^2)$ using ϵ for the term containing $\|U_j-\tilde{u}_j\|_{H^1_0(\Omega)}$ and $\epsilon=1$ otherwise:

$$\begin{aligned}\frac{1}{2}\frac{d}{dt}(\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}) \;\; \le \;\; & -\nu_1\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{H^1_0(\Omega)^3}+\frac{1}{2}\{\sum_{i=1}^{3}(\|(u_i-\tilde{u}_i)_t\|^2_{L^2(\Omega)}+\|U_i-\tilde{u}_i\|^2_{L^2(\Omega)})\\ & +\sum_{i=1}^{3}\sum_{j=1}^{3}(\epsilon\|U_j-\tilde{u}_j\|^2_{H^1_0(\Omega)}+L^2\epsilon^{-1}\|U_i-\tilde{u}_i\|^2_{L^2(\Omega)})\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}(\|\tilde{u}_j-u_j\|^2_{H^1_0(\Omega)}+\|U_i-\tilde{u}_i\|^2_{L^2(\Omega)})\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}(\|U_j-\tilde{u}_j\|^2_{L^2(\Omega)}+\|U_i-\tilde{u}_i\|^2_{L^2(\Omega)})\\ & +L\sum_{i=1}^{3}\sum_{j=1}^{3}(\|\tilde{u}_j-u_j\|^2_{L^2(\Omega)}+\|U_i-\tilde{u}_i\|^2_{L^2(\Omega)})\}.\end{aligned}$$

Collecting like terms, we have

$$\begin{aligned}\frac{d}{dt}(\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}) \;\; + \;\; & (2\nu_1-3\epsilon)\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{H^1_0(\Omega)^3} \le (1+3L^2\epsilon^{-1}+12L)\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}\\ & +\|(\mathbf{u}-\tilde{\mathbf{u}})_t\|^2_{L^2(\Omega)^3}+6L\|\tilde{\mathbf{u}}-\mathbf{u}\|^2_{H^1_0(\Omega)^3}\\ = \;\; & \|(\mathbf{u}-\tilde{\mathbf{u}})_t\|^2_{L^2(\Omega)^3}+C_1\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}+C_2\|\tilde{\mathbf{u}}-\mathbf{u}\|^2_{H^1_0(\Omega)^3}\end{aligned}$$

Now integrate with respect to t to get

$$\begin{aligned}\int_0^\tau\{\frac{d}{dt}(\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}) \;\; + \;\; & (2\nu_1-3\epsilon)\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{H^1_0(\Omega)^3}\}dt \le \int_0^\tau\{\|(\mathbf{u}-\tilde{\mathbf{u}})_t\|^2_{L^2(\Omega)^3}\\ & +C_1\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}+C_2\|\tilde{\mathbf{u}}-\mathbf{u}\|^2_{H^1_0(\Omega)^3}\}dt\end{aligned}$$

for $0 < \tau \leq \bar{T}$. Rearranging terms, we have, upon choosing $\epsilon < \frac{2}{3}\nu_1$,

$$\begin{aligned} 0 \leq \|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) \quad + & \quad (2\nu_1 - 3\epsilon)\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2((0,\tau),H^1_0(\Omega)^3)} \leq \|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(0) \\ & +\|(\mathbf{u}-\tilde{\mathbf{u}})_t\|^2_{L^2((0,\tau),L^2(\Omega)^3)} + C_2\|\tilde{\mathbf{u}}-\mathbf{u}\|^2_{L^2((0,\tau),H^1_0(\Omega)^3)} \\ & + \int_0^\tau C_1\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3} dt. \end{aligned}$$

Finally, we apply Gronwall's inequality and set $\delta = 2\nu_1 - 3\epsilon$ to get

$$\begin{aligned} \|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) \quad + & \quad \delta\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2((0,\tau),H^1_0(\Omega)^3)} \leq C_1^*\|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(0) \\ & +C_2^*\|(\mathbf{u}-\tilde{\mathbf{u}})_t\|^2_{L^2((0,\tau),L^2(\Omega)^3)} + C_3^*\|\tilde{\mathbf{u}}-\mathbf{u}\|^2_{L^2((0,\tau),H^1_0(\Omega)^3)}. \end{aligned}$$

■

We now present an error estimate for $\|\mathbf{U}-\mathbf{u}\|^2_{L^2(\Omega)^3}$.

Theorem 4.11 *Suppose Hypothesis 4.9 holds. Then for* $\tau \in [0, \bar{T}]$

$$\|\mathbf{U}-\mathbf{u}\|^2_{L^2(\Omega)^3}(\tau) \leq \hat{C}_1\|\mathbf{u}_0 - \mathbf{U}_0\|^2_{L^2(\Omega)^3} + \hat{C}_2 h^2\left(h^2\|\mathbf{u}_0\|^2_{H^2(\Omega)^3} + \|\mathbf{u}_t\|^2_{H^1_0(\Omega)^3} + \|\mathbf{u}\|^2_{H^2(\Omega)^3}\right)$$

where $\hat{C}_1, \hat{C}_2 > 0$ *are independent of* h *and* $\mathbf{u}_0$.

Proof. Using the triangle inequality, we have for each $\tau \in [0, \bar{T}]$

$$\|\mathbf{U}-\mathbf{u}\|^2_{L^2(\Omega)^3}(\tau) \leq \|\mathbf{U}-\tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) + \|\tilde{\mathbf{u}}-\mathbf{u}\|^2_{L^2(\Omega)^3}(\tau) \tag{4.30}$$

where $\tilde{\mathbf{u}}$ is the linear elliptic projection of $\mathbf{u}$ as defined by (4.26).

We know from Theorem 4.2 that for $u \in H^1_0(\Omega)$ and $\tilde{u} \in S^h$, the set of piecewise linear functions on the partition $\Delta_{[a,b]}$, we have the estimates

$$\|\tilde{u} - u\|_{L^2(\Omega)} \leq \tilde{C}h\|u\|_{H^1_0(\Omega)}$$

which extend easily to a linear elliptic system, that is,

$$\|\tilde{\mathbf{u}}-\mathbf{u}\|_{L^2(\Omega)^3} \leq Ch\|\mathbf{u}\|_{H^1_0(\Omega)^3}$$

We also know from Theorem 4.2 that for $u \in H^2$ and $\tilde{u} \in S^h$, the set of piecewise linear functions on the partition $\Delta_{[a,b]}$, we have the estimates

$$\begin{aligned} \|\tilde{u} - u\|_{L^2(\Omega)} &\leq \tilde{C}h^2\|u\|_{H^2(\Omega)} \\ \|\tilde{u} - u\|_{H^1_0(\Omega)} &\leq \tilde{C}h\|u\|_{H^2(\Omega)} \end{aligned}$$

which extend easily to a linear elliptic system, that is,

$$\begin{aligned}\|\tilde{\mathbf{u}} - \mathbf{u}\|_{L^2(\Omega)^3} &\leq Ch^2\|\mathbf{u}\|_{H^2(\Omega)^3}\\ \|\tilde{\mathbf{u}} - \mathbf{u}\|_{H_0^1(\Omega)^3} &\leq Ch\|\mathbf{u}\|_{H^2(\Omega)^3}.\end{aligned}$$

Thus, since $\mathbf{u} \in (H^2\Omega) \cap H_0^1(\Omega))^3$ and $\mathbf{u}_t \in H_0^1(\Omega))^3$, we have the following estimates,

$$\begin{aligned}\|\mathbf{U} - \tilde{\mathbf{u}}\|_{L^2(\Omega)^3}(0) &= \|\mathbf{U}_0 - \tilde{\mathbf{u}}_0\|_{L^2(\Omega)^3} = \|\mathbf{U}_0 - \mathbf{u}_0\|_{L^2(\Omega)^3} + \|\mathbf{u}_0 - \tilde{\mathbf{u}}_0\|_{L^2(\Omega)^3}\\ &\leq \|\mathbf{U}_0 - \mathbf{u}_0\|_{L^2(\Omega)^3} + Ch^2\|\mathbf{u}_0\|_{H^2(\Omega)^3} \quad (4.31)\\ \|(\tilde{\mathbf{u}} - \mathbf{u})_t\|_{L^2(\Omega)^3} &\leq Ch\|\mathbf{u}_t\|_{H^2(\Omega)^3} \quad (4.32)\\ \|\tilde{\mathbf{u}} - \mathbf{u}\|_{H_0^1(\Omega)^3} &\leq Ch\|\mathbf{u}\|_{H^2(\Omega)^3}. \quad (4.33)\end{aligned}$$

We now use the estimates (4.31)-(4.33) in the error estimate obtained from Theorem 4.10 for $\|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau)$ to get

$$\begin{aligned}\|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) &+ \delta\|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2((0,\tau),H_0^1(\Omega)^3)} \leq K_1^*(\|\mathbf{U}_0 - \mathbf{u}_0\|_{L^2(\Omega)^3} + Ch^2\|\mathbf{u}_0\|_{H^2(\Omega)^3})^2\\ &+K_2^* h^2\left(\|\mathbf{u}_t\|^2_{H^2(\Omega)^3} + \|\mathbf{u}\|^2_{H^2(\Omega)^3}\right). \quad (4.34)\end{aligned}$$

Using (4.34) and (4.32) in (4.30) we get

$$\begin{aligned}\|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) &+ \delta\|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2((0,\tau),H_0^1(\Omega)^3)} \leq K_1^*(\|\mathbf{U}_0 - \mathbf{u}_0\|_{L^2(\Omega)^3} + Ch^2\|\mathbf{u}_0\|_{H^2(\Omega)^3})^2\\ &+K_2^{**} h^2\left(\|\mathbf{u}_t\|^2_{H^2(\Omega)^3} + \|\mathbf{u}\|^2_{H^2(\Omega)^3}\right).\end{aligned}$$

Thus we have

$$\begin{aligned}\|\mathbf{U} - \tilde{\mathbf{u}}\|^2_{L^2(\Omega)^3}(\tau) \leq\ & \hat{C}_1\|\mathbf{U}_0 - \mathbf{u}_0\|^2_{L^2(\Omega)^3}\\ &+\hat{C}_2 h^2\left(h^2\|\mathbf{u}_0\|^2_{H^2(\Omega)^3} + \|\mathbf{u}_t\|^2_{H^2(\Omega)^3} + \|\mathbf{u}\|^2_{H^2(\Omega)^3}\right).\end{aligned}$$

■

4.4 A finite element algorithm for a system of nonlinear parabolic equations

In this section we develop a finite element algorithm to solve the initial value problem (2.44)-(2.52) by modifying the discretization techniques in Subsection 4.2.2. We start with the parabolic system:

$$\begin{aligned}w_t &= \epsilon_1^2 w_{xx} + v_x\\ \rho v_t &= \epsilon_2^2 v_{xx} + G''(w)w_x - \gamma\phi_x \quad (4.35)\\ \beta\phi_t &= \epsilon_3^2\phi_{xx} + \gamma w - \alpha\phi\end{aligned}$$

where $x \in [a,b]$ and $t \in (0,T)$. We wish to create a method that will solve a system with any combination of Dirichlet and Neumann boundary conditions. We choose the following boundary conditions as an example:

$$w(t,a) = \alpha_w(t), \qquad w_x(t,b) = \beta_w(t) \tag{4.36}$$

$$v_x(t,a) = \alpha_v(t), \qquad v(t,b) = \beta_v(t) \tag{4.37}$$

$$\phi(t,a) = \alpha_\phi(t), \qquad \phi_x(t,b)(t) = \beta_\phi(t) \tag{4.38}$$

and initial conditions

$$\begin{aligned} w(0,x) &= w_0(x) \\ v(0,x) &= v_0(x) \\ \phi(0,x) &= \phi_0(x) \end{aligned}$$

The partition in the x variable is $\Delta_{[a,b]} = \{a = x_0 < x_1 < \cdots < x_i < \cdots < x_{N-1} < x_N = b\}$, where $x_i = a + ih, 0 \le i \le N$ and $h = \frac{b-a}{N}$. We write out the weak formulation for the system (4.35):

$$\begin{aligned} \langle w_t, \tilde{w} \rangle &= \langle \epsilon_1^2 w_{xx}, \tilde{w} \rangle + \langle v_x, \tilde{w} \rangle \\ \langle \rho v_t, \tilde{v} \rangle &= \langle \epsilon_2^2 v_{xx}, \tilde{v} \rangle + \langle G''(w) w_x, \tilde{v} \rangle - \langle \gamma \phi_x, \tilde{v} \rangle \\ \langle \beta \phi_t, \tilde{\phi} \rangle &= \langle \epsilon_3^2 \phi_{xx}, \tilde{\phi} \rangle + \langle \gamma w, \tilde{\phi} \rangle - \langle \alpha \phi, \tilde{\phi} \rangle \end{aligned}$$

Here $\tilde{w}, \tilde{\phi} \in \{u \in H^1(a,b) : u(a) = 0\}$ and $\tilde{v} \in \{u \in H^1(a,b) : u(b) = 0\}$. Integrating by parts, we have

$$\langle w_t, \tilde{w} \rangle = \langle -\epsilon_1^2 w_x, \tilde{w}_x \rangle + \epsilon_1^2 w_x \tilde{w}|_a^b + \langle v_x, \tilde{w} \rangle \tag{4.39}$$

$$\langle \rho v_t, \tilde{v} \rangle = \langle -\epsilon_2^2 v_x, \tilde{v}_x \rangle + \epsilon_2^2 v_x \tilde{v}|_a^b + \langle G''(w) w_x, \tilde{v} \rangle - \langle \gamma \phi_x, \tilde{v} \rangle \tag{4.40}$$

$$\langle \beta \phi_t, \tilde{\phi} \rangle = \langle -\epsilon_3^2 \phi_x, \tilde{\phi}_x \rangle + \epsilon_3^2 \phi_x \tilde{\phi}|_a^b + \langle \gamma w, \tilde{\phi} \rangle - \langle \alpha \phi, \tilde{\phi} \rangle. \tag{4.41}$$

We use the space of piecewise linear functions on $[a,b]$ to approximate the solution to the system (4.35). Since the boundary conditions (4.36) of w are nonhomogeneous, the finite element spaces S_h^w, S_h^v and S_h^ϕ are the space $\tilde{S}_h$ defined by (4.10). We denote the basis of hat functions for S_h^w by $\{\chi_j\}_{j=0}^{N_w}$, where $\chi_j = \psi_j, 0 \le j \le N_w = N$ where the functions ϕ_j are defined by (4.4), (4.11) and (4.12). Similarly, we denote the basis of hat functions for S_h^v and S_h^ϕ by $\{\eta_j\}_{j=0}^{N_w}$ and $\{\xi_j\}_{j=0}^{N_w}$, respectively, where $\eta_j = \psi_j, 0 \le j \le N_v = N$, and $\xi_j = \psi_j, 0 \le j \le N_\phi = N$. The choice of boundary conditions yields the space of test functions

$$\hat{\mathbf{S}} = \left\{ \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \end{bmatrix} : y_1 \in \hat{S}_h^w, y_2 \in \hat{S}_h^v, y_3 \in \hat{S}_h^\phi \right\}$$

where $\hat{S}_h^w, \hat{S}_h^v$ and $\hat{S}_h^\phi$ are subspaces of $\tilde{S}_h$. We identify each space by its basis,

$$\hat{S}_h^w = \{\hat{\chi}_i\}_{i=1}^{N_w} \tag{4.42}$$

$$\hat{S}_h^v = \{\hat{\eta}_i\}_{i=1}^{N_v} \tag{4.43}$$

$$\hat{S}_h^\phi = \{\hat{\xi}_i\}_{i=1}^{N_\phi} \tag{4.44}$$

where $\tilde{\chi}_j = \psi_j$ for $1 \leq N_w$, $\tilde{\eta}_j = \psi_{j-1}$ for $1 \leq N_v$ and $\tilde{\xi}_j = \psi_j$ for $1 \leq N_\phi$. We note that the subscripts have a direct correlation to the boundary conditions (4.36)-(4.38), that is, we take our subspaces (4.42)-(4.44) to be those which corresponds to the grid points where the solutions w, v and ϕ are unknown.

Using (4.42)-(4.44) as test functions, we define the semidiscrete finite element solutions for (4.39)-(4.41) are, as the functions

$$w_h(x,t) = \alpha_w \chi_0(x) + \sum_{j=1}^{N_w} w_{h,j}(t)\chi_j(x) \tag{4.45}$$

$$v_h(x,t) = \sum_{j=0}^{N_v-1} v_{h,j}(t)\eta_j(x) + \beta_v \eta_{N_v}(x) \tag{4.46}$$

$$\phi_h(x,t) = \alpha_\phi \xi_0(x) + \sum_{j=1}^{N_\phi} \phi_{h,j}(t)\xi_j(x). \tag{4.47}$$

which satisfy

$$\begin{array}{rcl}
\langle w_{h,t}, \hat{\chi}_i \rangle & = & \langle -\epsilon_1^2 w_{h,x}, \hat{\chi}_{i,x} \rangle + \epsilon_1^2 w_{h,x}\hat{\chi}_i|_a^b + \langle v_{h,x}, \hat{\chi}_i \rangle \\
 & & i = 1, \cdots, N_w \\
\langle \rho v_{h,t}, \hat{\eta}_i \rangle & = & \langle -\epsilon_2^2 v_{h,x}, \hat{\eta}_{i,x} \rangle + \epsilon_2^2 v_{h,x}\hat{\eta}_i|_a^b + \langle G''(w_h)w_{h,x}, \hat{\eta}_i \rangle - \langle \gamma \phi_{h,x}, \hat{\eta}_i \rangle \\
 & & i = 1, \cdots, N_v \\
\langle \beta \phi_{h,t}, \hat{\xi}_i \rangle & = & \langle -\epsilon_3^2 \phi_{h,x}, \hat{\xi}_{i,x} \rangle + \epsilon_3^2 \phi_{h,x}\hat{\xi}_i|_a^b + \langle \gamma w_h, \hat{\xi}_i \rangle - \langle \alpha \phi_h, \hat{\xi}_i \rangle \\
 & & i = 1, \cdots, N_\phi
\end{array} \tag{4.48}$$

and

$$\begin{bmatrix} w_h(0) \\ v_h(0) \\ \phi_h(0) \end{bmatrix} = \begin{bmatrix} w_h^0 \\ v_h^0 \\ \phi_h^0 \end{bmatrix}$$

where $\begin{bmatrix} w_h^0 \\ v_h^0 \\ \phi_h^0 \end{bmatrix} \in \mathbf{S}_h$ is an approximation of $\begin{bmatrix} w_0 \\ v_0 \\ \phi_0 \end{bmatrix}$.

In the following discussion we use the prime notation to denote a derivative with respect to the x variable, i.e., $\chi' = \chi_x$. Using (4.45)-(4.47) in (4.48), we have

$$\begin{array}{rcl}
\sum_{j=1}^{N_w} \langle w_{h,j,t}\chi_j, \hat{\chi}_i \rangle + \langle w_{h,0,t}\chi_0, \hat{\chi}_i \rangle & = & \sum_{j=1}^{N_w} \langle -\epsilon_1^2 w_{h,j}\chi_j', \hat{\chi}_i' \rangle + \langle -\epsilon_1^2 w_{h,0}\chi_0', \hat{\chi}_i' \rangle \\
 & + & \epsilon_1^2 w_{h,N_w}\chi_{N_w}'\hat{\chi}_i(b) - \epsilon_1^2 w_{h,0}\chi_0'(a)\hat{\chi}_i(a) \\
 & + & \sum_{j=0}^{N_v-1} \langle v_{h,j}\eta_j', \hat{\chi}_i \rangle + \langle v_{h,N_v}\eta_{N_v}', \hat{\chi}_i \rangle \\
 & & i = 1, \cdots, N_w
\end{array} \tag{4.49}$$

$$
\begin{aligned}
\sum_{j=0}^{N_v-1} \langle \rho v_{h,j,t} \eta_j, \hat{\eta}_i \rangle + \langle \rho v_{h,N_v,t} \eta_{N_v}, \hat{\chi}_i \rangle &= \sum_{j=0}^{N_v-1} \langle -\epsilon_2^2 v_{h,j} \eta_j', \hat{\eta}_i' \rangle + \langle -\epsilon_2^2 v_{h,N_v,x} \eta_{N_v}', \hat{\eta}_i' \rangle \\
&+ \epsilon_2^2 v_{h,N_v} \eta_{N_v}'(b) \hat{\chi}_i(b) - \epsilon_2^2 v_{h,0} \eta_0'(a) \hat{\eta}_i(a) \\
&+ \sum_{j=1}^{N_w} \langle G''(w_h) w_{h,j} \chi_j', \hat{\eta}_i \rangle + \langle G''(w_h) w_{h,0} \chi_0', \hat{\eta}_i \rangle \\
&- \sum_{j=1}^{N_\phi} \langle \gamma \phi_{h,j} \xi_j', \hat{\eta}_i \rangle - \langle \gamma \phi_{h,0} \xi_0', \hat{\eta}_i \rangle \\
&\qquad\qquad i = 1, \cdots, N_v
\end{aligned} \tag{4.50}
$$

$$
\begin{aligned}
\sum_{j=1}^{N_\phi} \langle \beta \phi_{h,j,t} \xi_j, \hat{\xi}_i \rangle + \langle \beta \phi_{h,0,t} \xi_0, \hat{\xi}_i \rangle &= \sum_{j=1}^{N_\phi} \langle -\epsilon_3^2 \phi_{h,j} \xi_j', \hat{\xi}_i' \rangle + \langle -\epsilon_3^2 \phi_{h,0,x} \xi_0', \hat{\xi}_i' \rangle \\
&+ \epsilon_3^2 \phi_{h,N_\phi} \xi_{N_\phi}'(b) \hat{\xi}_i(b) - \epsilon_3^2 \phi_{h,0} \xi_0'(a) \hat{\xi}_i(a) \\
&+ \sum_{j=1}^{N_w} \langle \gamma w_{h,j} \chi_j, \hat{\xi}_i \rangle + \langle \gamma w_{h,0} \chi_0, \hat{\xi}_i \rangle \\
&- \sum_{j=1}^{N_\phi} \langle \alpha \phi_{h,j} \xi_j, \hat{\xi}_i \rangle - \langle \alpha \phi_{h,0} \xi_0, \hat{\xi}_i \rangle \\
&\qquad\qquad i = 1, \cdots, N_\phi.
\end{aligned} \tag{4.51}
$$

Let y, z represent any of the basis functions of a finite dimensional subspace of $H_0^1(a, b)$, we define the matrices, $M_a^{y,z}$, $B_a^{y,z}$ and $S_a^{y,z}$, of inner products componentwise by

$$
\begin{aligned}
[M_a^{y,z}]_{i,j} &= \langle a(x) y_j, z_i \rangle \\
[B_a^{y,z}]_{i,j} &= \langle a(x) y_j', z_i \rangle \\
[S_a^{y,z}]_{i,j} &= \langle a(x) y_j', z_i' \rangle,
\end{aligned}
$$

$1 \le i \le N_z, 1 \le j \le N_y$ or $0 \le j \le N_y - 1$ as the case may be. Note that M is a mass matrix, S is a stiffness matrix and B is a mixed matrix, that is, a matrix of mixed derivatives. Let $\mathbf{b}_{1,t} = \begin{bmatrix} \langle w_{h,0,t} \chi_0, \hat{\chi}_1 \rangle \\ \vdots \\ \langle w_{h,0,t} \chi_0, \hat{\chi}_{N_w} \rangle \end{bmatrix}$, $\mathbf{b}_{2,t} = \begin{bmatrix} \langle v_{h,N_v,t} \eta_{N_v}, \hat{\eta}_1 \rangle \\ \vdots \\ \langle v_{h,N_v,t} \eta_{N_v}, \hat{\eta}_{N_v} \rangle \end{bmatrix}$ and $\mathbf{b}_{3,t} = \begin{bmatrix} \langle \phi_{h,0,t} \xi_0, \hat{\xi}_1 \rangle \\ \vdots \\ \langle \phi_{h,0,t} \xi_0, \hat{\xi}_{N_\phi} \rangle \end{bmatrix}$ be the contributions of the boundary term on the left hand side of the equations (4.49)-(4.51). Let

$$
\mathbf{c}_1 = \begin{bmatrix}
\langle -\epsilon_1^2 w_{h,0} \chi_0', \hat{\chi}_1' \rangle & + & \epsilon_1^2 w_{h,N_w} \chi_{N_w}'(b) \hat{\chi}_1'(b) - \epsilon_1^2 w_{h,0} \chi_0'(a) \hat{\chi}_1'(a) \\
 & & + \langle v_{h,N_v} \eta_0', \hat{\chi}_1 \rangle \\
 & & \vdots \\
\langle -\epsilon_1^2 w_{h,0} \chi_0', \hat{\chi}_{N_w}' \rangle & + & \epsilon_1^2 w_{h,N_w} \chi_{N_w}'(b) \hat{\chi}_{N_w}'(b) - \epsilon_1^2 w_{h,0} \chi_0'(a) \hat{\chi}_{N_w}'(a) \\
 & & + \langle v_{h,N_v} \eta_0', \hat{\chi}_{N_w} \rangle
\end{bmatrix}
$$

$$\mathbf{c}_2 = \begin{bmatrix} \langle -\epsilon_2^2 v_{h,N_v}\eta'_{N_v}, \hat{\eta}'_1\rangle & + & \epsilon_2^2 v_{h,N_v}\eta'_{N_v}(b)\hat{\eta}_1(b) - \epsilon_2^2 v_{h,N_v}\eta'_{N_v}(a)\hat{\eta}_1(a) \\ & & +\langle G''(w_h)w_{h,0}\chi'_0, \hat{\eta}'_1\rangle - \langle \gamma\phi_{h,0}\xi'_0, \hat{\eta}_1\rangle \\ & & \vdots \\ \langle -\epsilon_2^2 v_{h,N_v}\eta'_{N_v}, \hat{\eta}'_{N_v}\rangle & + & \epsilon_2^2 v_{h,N_v}\eta'_{N_v}(b)\hat{\eta}_{N_v}(b) - \epsilon_2^2 v_{h,N_v}\eta'_{N_v}(a)\hat{\eta}_{N_v}(a) \\ & & +\langle G''(w_h)w_{h,0}\chi'_0, \hat{\eta}_{N_v}\rangle - \langle \gamma\phi_{h,0}\xi'_0, \hat{\eta}_{N_v}\rangle \end{bmatrix}$$

$$\mathbf{c}_3 = \begin{bmatrix} \langle -\epsilon_3^2 \phi_{h,0}\xi'_0, \hat{\xi}'_1\rangle & + & \epsilon_3^2 \phi_{h,N_{phi}}\xi'_{N_\phi}(b)\hat{\xi}_1(b) - \epsilon_3^2 \phi_{h,0}\xi'_0(a)\hat{\xi}_1(a) \\ & & +\langle \gamma w_{h,0}\chi_0, \hat{\xi}_1\rangle - \langle \alpha\phi_{h,0}\xi_0, \hat{\xi}_1\rangle \\ & & \vdots \\ \langle -\epsilon_3^2 \phi_{h,0}\xi'_0, \hat{\xi}'_{N_\phi}\rangle & + & \epsilon_3^2 \phi_{h,N_{phi}}\xi'_{N_\phi}(b)\hat{\xi}_{N_\phi}(b) - \epsilon_3^2 \phi_{h,0}\xi'_0(a)\hat{\xi}_{N_\phi}(a) \\ & & +\langle \gamma w_{h,0}\chi_0, \hat{\xi}_{N_\phi}\rangle - \langle \alpha\phi_{h,0}\xi_0, \hat{\xi}_{N_\phi}\rangle \end{bmatrix}$$

be the contributions of the known boundary term on the right hand side of the above equations (4.49)-(4.51). Also, let $\mathbf{w}_h(t) = \begin{bmatrix} w_{h,1}(t) \\ \vdots \\ w_{h,N_w}(t) \end{bmatrix}$, $\mathbf{v}_h(t) = \begin{bmatrix} v_{h,0}(t) \\ \vdots \\ w_{h,N_v-1}(t) \end{bmatrix}$ and $\phi_{\mathbf{h}}(\mathbf{t}) = \begin{bmatrix} \phi_{h,1}(t) \\ \vdots \\ \phi_{h,N_\phi}(t) \end{bmatrix}$. Writing the finite element equations in matrix form using the above notation, we have

$$\begin{aligned} M_1^{\chi,\hat{\chi}}\mathbf{w}_{h,t} + S_{\epsilon_1^2}^{\chi,\hat{\chi}}\mathbf{w}_h + \mathbf{b}_{1,t} &= B_1^{\eta,\hat{\chi}}\mathbf{v}_h + \mathbf{c}_1 \\ M_\rho^{\eta,\hat{\eta}}\mathbf{v}_{h,t} + S_{\epsilon_2^2}^{\eta,\hat{\eta}}\mathbf{v}_h + \mathbf{b}_{2,t} &= B_{G''(w_h)}^{\chi,\hat{\eta}}\mathbf{w}_h - B_\gamma^{\xi,\hat{\eta}}\phi_{\mathbf{h}} + \mathbf{c_2} \\ M_\beta^{\xi,\hat{\xi}}\phi_{\mathbf{h,t}} + \mathbf{S}_{\epsilon_\mathbf{3}^\mathbf{2}}^{\xi,\hat{\xi}}\phi_{\mathbf{h}} + \mathbf{b_{3,t}} &= M_\gamma^{\chi,\hat{\xi}}\mathbf{w}_h - M_\alpha^{\xi,\hat{\xi}}\phi_{\mathbf{h}} + \mathbf{c_3}. \end{aligned}$$

For each time t, we set $\mathbf{u}_h(t) = \begin{bmatrix} \mathbf{w}_h(t) \\ \mathbf{v}_h(t) \\ \phi_{\mathbf{h}}(\mathbf{t}) \end{bmatrix}$. Then the above system of matrix equations can be written as one $(N_w + N_v + N_\phi) \times (N_w + N_v + N_\phi)$ matrix equation for each time t:

$$\begin{bmatrix} M_1^{\chi,\hat{\chi}} & \mathbf{0}_{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ \mathbf{0}_{\eta,\hat{\chi}} & M_\rho^{\eta,\hat{\eta}} & \mathbf{0}_{\eta,\hat{\xi}} \\ \mathbf{0}_{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & M_\beta^{\xi,\hat{\xi}} \end{bmatrix} \mathbf{u}_{h,t} + \begin{bmatrix} \mathbf{b}_{1,t} \\ \mathbf{b}_{2,t} \\ \mathbf{b}_{3,t} \end{bmatrix} = \begin{bmatrix} -S_{\epsilon_1^2}^{\chi,\hat{\chi}} & B_1^{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ B_{G''(w_h)}^{\eta,\hat{\chi}} & -S_{\epsilon_2^2}^{\eta,\hat{\eta}} & -B_\gamma^{\eta,\hat{\xi}} \\ M_\gamma^{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & -S_{\epsilon_3^2}^{\xi,\hat{\xi}} - M_\alpha^{\xi,\hat{\xi}} \end{bmatrix} \mathbf{u}_h + \begin{bmatrix} \mathbf{c}_1 \\ \mathbf{c}_2 \\ \mathbf{c}_3 \end{bmatrix}.$$

We now use the Crank-Nicolson difference method to determine $\mathbf{u}_{h,t}(t_n)$ where $t_n = n\tau$ where τ is the time step. Recall from Subsection 4.2.2, the Crank-Nicolson-Galerkin method discretizes the above equation symmetrically about the point $t_{n-\frac{1}{2}} = (n - \frac{1}{2})\tau$. We use the following substitutions in the above matrix equation

$$\begin{aligned}\mathbf{u}_{h,t}^{n-\frac{1}{2}} &= \tau^{-1}(\mathbf{u}_h^n - \mathbf{u}_h^{n-1})\\ \mathbf{u}_h^{n-\frac{1}{2}} &= \frac{1}{2}(\mathbf{u}_h^n + \mathbf{u}_h^{n-1}).\end{aligned}$$

We now have

$$\begin{bmatrix} M_1^{\chi,\hat{\chi}} & \mathbf{0}_{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ \mathbf{0}_{\eta,\hat{\chi}} & M_\rho^{\eta,\hat{\eta}} & \mathbf{0}_{\eta,\hat{\xi}} \\ \mathbf{0}_{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & M_\beta^{\xi,\hat{\xi}} \end{bmatrix} \tau^{-1}(\mathbf{u}_h^n - \mathbf{u}_h^{n-1}) + \tau^{-1}\left(\begin{bmatrix}\mathbf{b}_1^n\\ \mathbf{b}_2^n\\ \mathbf{b}_3^n\end{bmatrix} - \begin{bmatrix}\mathbf{b}_1^{n-1}\\ \mathbf{b}_2^{n-1}\\ \mathbf{b}_3^{n-1}\end{bmatrix}\right) =$$
$$\begin{bmatrix} -S_{\epsilon_1^2}^{\chi,\hat{\chi}} & B_1^{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ B_{G''(w_h^n)}^{\eta,\hat{\chi}} & -S_{\epsilon_2^2}^{\eta,\hat{\eta}} & -B_\gamma^{\eta,\hat{\xi}} \\ M_\gamma^{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & -S_{\epsilon_3^2}^{\xi,\hat{\xi}} - M_\alpha^{\xi,\hat{\xi}} \end{bmatrix} \frac{1}{2}(\mathbf{u}_h^n + \mathbf{u}_h^{n-1}) + \frac{1}{2}\left(\begin{bmatrix}\mathbf{c}_1^n\\ \mathbf{c}_2^n\\ \mathbf{c}_3^n\end{bmatrix} + \begin{bmatrix}\mathbf{c}_1^{n-1}\\ \mathbf{c}_2^{n-1}\\ \mathbf{c}_3^{n-1}\end{bmatrix}\right)$$

And finally, solving for $\mathbf{u}_h^n$, we have

$$\left(\tau^{-1}\begin{bmatrix} M_1^{\chi,\hat{\chi}} & \mathbf{0}_{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ \mathbf{0}_{\eta,\hat{\chi}} & M_\rho^{\eta,\hat{\eta}} & \mathbf{0}_{\eta,\hat{\xi}} \\ \mathbf{0}_{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & M_\beta^{\xi,\hat{\xi}} \end{bmatrix} - \tfrac{1}{2}\begin{bmatrix} -S_{\epsilon_1^2}^{\chi,\hat{\chi}} & B_1^{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ B_{G''(w_h^n)}^{\eta,\hat{\chi}} & -S_{\epsilon_2^2}^{\eta,\hat{\eta}} & -B_\gamma^{\eta,\hat{\xi}} \\ M_\gamma^{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & -S_{\epsilon_3^2}^{\xi,\hat{\xi}} - M_\alpha^{\xi,\hat{\xi}} \end{bmatrix}\right)\mathbf{u}_h^n =$$
$$\left(\tau^{-1}\begin{bmatrix} M_1^{\chi,\hat{\chi}} & \mathbf{0}_{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ \mathbf{0}_{\eta,\hat{\chi}} & M_\rho^{\eta,\hat{\eta}} & \mathbf{0}_{\eta,\hat{\xi}} \\ \mathbf{0}_{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & M_\beta^{\xi,\hat{\xi}} \end{bmatrix} + \tfrac{1}{2}\begin{bmatrix} -S_{\epsilon_1^2}^{\chi,\hat{\chi}} & B_1^{\chi,\hat{\eta}} & \mathbf{0}_{\chi,\hat{\xi}} \\ B_{G''(w_h^n)}^{\eta,\hat{\chi}} & -S_{\epsilon_2^2}^{\eta,\hat{\eta}} & -B_\gamma^{\eta,\hat{\xi}} \\ M_\gamma^{\xi,\hat{\chi}} & \mathbf{0}_{\xi,\hat{\eta}} & -S_{\epsilon_3^2}^{\xi,\hat{\xi}} - M_\alpha^{\xi,\hat{\xi}} \end{bmatrix}\right)\mathbf{u}_h^{n-1} +$$
$$\tfrac{1}{2}\begin{bmatrix}\mathbf{c}_1^{n-1}\\ \mathbf{c}_2^{n-1}\\ \mathbf{c}_3^{n-1}\end{bmatrix} + \tau^{-1}\begin{bmatrix}\mathbf{b}_1^{n-1}\\ \mathbf{b}_2^{n-1}\\ \mathbf{b}_3^{n-1}\end{bmatrix} - \tau^{-1}\begin{bmatrix}\mathbf{b}_1^n\\ \mathbf{b}_2^n\\ \mathbf{b}_3^n\end{bmatrix} + \tfrac{1}{2}\begin{bmatrix}\mathbf{c}_1^n\\ \mathbf{c}_2^n\\ \mathbf{c}_3^n\end{bmatrix} \tag{4.52}$$

The last detail to consider is the nonlinear function $G''(w_h^n)$. We use the substitution $w_h^n = \frac{3}{2}w_h^{n-1} - \frac{1}{2}w_h^{n-2}$ for $n \geq 2$. This requires knowing w_h^1 in advance. To do so, we first solve the equation

$$\left(\tau^{-1}\begin{bmatrix} M_1^{\chi,\hat\chi} & \mathbf{0}_{\chi,\hat\eta} & \mathbf{0}_{\chi,\hat\xi} \\ \mathbf{0}_{\eta,\hat\chi} & M_\rho^{\eta,\hat\eta} & \mathbf{0}_{\eta,\hat\xi} \\ \mathbf{0}_{\xi,\hat\chi} & \mathbf{0}_{\xi,\hat\eta} & M_\beta^{\xi,\hat\xi} \end{bmatrix} - \frac{1}{2}\begin{bmatrix} -S_{\epsilon_1^2}^{\chi,\hat\chi} & B_1^{\chi,\hat\eta} & \mathbf{0}_{\chi,\hat\xi} \\ B_{G''(w_h^0)}^{\eta,\hat\chi} & -S_{\epsilon_2^2}^{\eta,\hat\eta} & -B_\gamma^{\eta,\hat\xi} \\ M_\gamma^{\xi,\hat\chi} & \mathbf{0}_{\xi,\hat\eta} & -S_{\epsilon_3^2}^{\xi,\hat\xi} - M_\alpha^{\xi,\hat\xi} \end{bmatrix}\right)\mathbf{u}_h^{1,0} =$$

$$\left(\tau^{-1}\begin{bmatrix} M_1^{\chi,\hat\chi} & \mathbf{0}_{\chi,\hat\eta} & \mathbf{0}_{\chi,\hat\xi} \\ \mathbf{0}_{\eta,\hat\chi} & M_\rho^{\eta,\hat\eta} & \mathbf{0}_{\eta,\hat\xi} \\ \mathbf{0}_{\xi,\hat\chi} & \mathbf{0}_{\xi,\hat\eta} & M_\beta^{\xi,\hat\xi} \end{bmatrix} + \frac{1}{2}\begin{bmatrix} -S_{\epsilon_1^2}^{\chi,\hat\chi} & B_1^{\chi,\hat\eta} & \mathbf{0}_{\chi,\hat\xi} \\ B_{G''(w_h^0)}^{\eta,\hat\chi} & -S_{\epsilon_2^2}^{\eta,\hat\eta} & -B_\gamma^{\eta,\hat\xi} \\ M_\gamma^{\xi,\hat\chi} & \mathbf{0}_{\xi,\hat\eta} & -S_{\epsilon_3^2}^{\xi,\hat\xi} - M_\alpha^{\xi,\hat\xi} \end{bmatrix}\right)\mathbf{u}_h^{0} +$$

$$\frac{1}{2}\begin{bmatrix} \mathbf{c}_1^0 \\ \mathbf{c}_2^0 \\ \mathbf{c}_3^0 \end{bmatrix} + \tau^{-1}\begin{bmatrix} \mathbf{b}_1^0 \\ \mathbf{b}_2^0 \\ \mathbf{b}_3^0 \end{bmatrix} - \tau^{-1}\begin{bmatrix} \mathbf{b}_1^1 \\ \mathbf{b}_2^1 \\ \mathbf{b}_3^1 \end{bmatrix} + \frac{1}{2}\begin{bmatrix} \mathbf{c}_1^1 \\ \mathbf{c}_2^1 \\ \mathbf{c}_3^1 \end{bmatrix}$$

for $\mathbf{u}_h^{1,0}$. We then use the substitution $w_h^1 = \frac{1}{2}(w_h^{1,0} + w_h^0)$ in $G''(w_h^1)$ to solve equation (4.52) for $\mathbf{u}_h^1$.

We now show that the hypotheses for Theorems 4.10 and 4.11 are satisfied for the above algorithm using homogeneous Dirichlet boundary conditions. Let $\mathbf{u} = \begin{bmatrix} w \\ v \\ \phi \end{bmatrix}$. We begin by rewriting the system (4.35) as

$$\begin{bmatrix} w_t \\ v_t \\ \phi_t \end{bmatrix} = \begin{bmatrix} \epsilon_1^2 w_{xx} \\ \epsilon_2^2 v_{xx} \\ \epsilon_3^2 \phi_{xx} \end{bmatrix} + \begin{bmatrix} f_1(\mathbf{u},\mathbf{u}_x) \\ f_2(\mathbf{u},\mathbf{u}_x) \\ f_3(\mathbf{u},\mathbf{u}_x) \end{bmatrix}, \quad (x,t) \in [a,b]\times(0,T) \tag{4.53}$$

$$\begin{bmatrix} w(a,t) \\ v(a,t) \\ \phi(a,t) \end{bmatrix} = \begin{bmatrix} w(b,t) \\ v(b,t) \\ \phi(b,t) \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ 0 \end{bmatrix} \quad t \in (0,T) \tag{4.54}$$

$$\begin{bmatrix} w(x,0) \\ v(x,0) \\ \phi(x,0) \end{bmatrix} = \begin{bmatrix} w_0(x) \\ v_0(x) \\ \phi_0(x) \end{bmatrix} \quad x \in \Omega. \tag{4.55}$$

The bilinear form, $\mathbf{B}$, associated with the above problem is

$$\mathbf{B}(\mathbf{u},\mathbf{v}) = \langle \epsilon_1^2 u_{1,x}, v_{1,x}\rangle + \langle \epsilon_2^2 u_{2,x}, v_{2,x}\rangle + \langle \epsilon_3^2 u_{3,x}, v_{3,x}\rangle$$

for all $\mathbf{u},\mathbf{v} \in H_0^1(a,b)^3$. We define the function $\mathbf{f} : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ by

$$\mathbf{f}(\mathbf{u},\mathbf{v}) = \begin{bmatrix} f_1(\mathbf{u},\mathbf{v}) \\ f_2(\mathbf{u},\mathbf{v}) \\ f_3(\mathbf{u},\mathbf{v}) \end{bmatrix} = \begin{bmatrix} v_2 \\ g(u_1)v_1 - \gamma v_3 \\ \gamma u_1 - \alpha u_3 \end{bmatrix}. \tag{4.56}$$

Let $\mathbf{u}_0 \in H^2(\Omega) \cap H_0^1(\Omega)$. We note that since $\epsilon_i^2 > 0, i = 1, 2, 3$, the $\mathbf{B}$ satisfies Hypothesis 4.9. By Theorem 3.1, the unique solution, $\mathbf{u}$, of the initial value problem with homogeneous boundary conditions also satisfies Hypothesis 4.9. To apply Theorems 4.10 and 4.11 we need only show $f_i, i = 1, 2, 3$ defined by (4.56) are locally Lipschitz on $\mathbb{R}^3 \times \mathbb{R}^3$.

Lemma 4.12 *Suppose that $g : \mathbb{R} \to \mathbb{R}$ is locally Lipschitz. Then $f_i : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{R}$ are also locally Lipschitz.*

Proof. Let D be a bounded subset of $\mathbb{R}^3$. We show that f_2 is Lipschitz in both $\mathbf{u}$ and $\mathbf{v}$ on D, noting that the cases of f_1 and f_3 are trivial.

Let $\mathbf{u}, \mathbf{u}^*, \mathbf{v}, \mathbf{v}^* \in D$. Then

$$|f_2(\mathbf{u}, \mathbf{v}) - f_2(\mathbf{u}^*, \mathbf{v})| = |v_1|\ |g(u_1) - g(u_1^*)| \leq L|v_1||u_1 - u_1^*| \leq LC\|\mathbf{u} - \mathbf{u}^*\|_{l^2}$$

since g is locally Lipschitz and D is bounded. Similarly, since g is bounded on on a bounded domain,

$$|f_2(\mathbf{u}, \mathbf{v}) - f_2(\mathbf{u}, \mathbf{v}^*)| = |g(u_1)|\ |v_1 - v_1^*| \leq M|v_1 - v_1^*| \leq M\|\mathbf{u} - \mathbf{u}^*\|_{l^2}.$$

■

Corollary 4.13 *Let $g : \mathbb{R} \to \mathbb{R}$ be a triple-well function defined by (2.40) for some fixed $\theta_0 > 0$. Let $\mathbf{u}_0 = \begin{bmatrix} w_0 \\ v_0 \\ \phi_0 \end{bmatrix} \in H^2(\Omega)^3 \cap H_0^1(\Omega)^3$. Suppose we solve the initial boundary value problem (4.53)-(4.55) using the above Crank-Nicolson-Galerkin method where $\mathbf{f}$ is defined by (4.56). Then the error estimates from Theorems 4.10 and 4.11 hold.*

The proof of Corollary 4.13 follows immediately from Lemma 4.12.

We note that the above algorithm is derived for non-constant Neumann and Dirichlet boundary conditions. We show convergence for the non-constant boundary conditions through numerical experiments in Chapter 5. We do not show error estimates for the fully discretized algorithm, yet we assume that it is possible to show convergence. Our numerical calculations in Chapter 5 suggest that this is the case.

Chapter 5

Numerical Computations for the Temperature Independent Model

5.1 Introduction

In this chapter we present results of numerical experiments using the Crank-Nicolson-Galerkin method developed in Chapter 4. We see that our system develops sharp phase boundaries that move in ways that correspond well with a number of experimental observations.

5.2 Numerical computations

We first present computational evidence that the Crank-Nicolson-Galerkin finite element algorithm developed in Section 4.3 converges as the number of time and space steps increase. We then present the results of several numerical experiments.

The error estimate (4.11) established in Section 4.4 is for constant Dirichlet boundary conditions. In the all our computations we use constant Neumann boundary conditions in conjunction with a non-constant Dirichlet boundary condition. We have not derived error estimates for this situation. However, we do test for convergence computationally. Choosing nonhomogeneous boundary and initial conditions which correspond to a known exact solution, we solved the temperature independent system (2.44)-(2.46) using the algorithm developed in Chapter 4. We refine the number of space steps, N_x, and the number of time steps, N_t and look at the l^2 error, $e = \mathbf{u} - \mathbf{u}_h^N$, at time $t = t_N$ (see Table 5.1). We observe that the error decreases at least linearly as N_x and N_t increase provided $N_t \geq N_x$. This type of error behavior is consistent with the Crank-Nicolson-Galerkin method, see e.g. [95].

We now turn to the numerical experiments. Let us first describe the physical experi-

Table 5.1: l^2 Error for non-constant boundary conditions ($\times 10^{-3}$)

	$N_t = 20$	$N_t = 40$	$N_t = 80$
$N_x = 20$	4.5973	1.5390	1.3268
$N_x = 40$	7.1163	1.6178	0.54244
$N_x = 80$	10.665	2.5179	0.57030

ment. Consider a bar of unit length and uniform cross section of a material which has three natural solid phases, p_1, p_2 and p_3. Associated with this material is a symmetric triple-well potential, $G(w)$. The local minima, w_1 and w_3, of the outer wells correspond to phase, p_1 and p_3, respectively. The local minima, w_2, of the inner well corresponds to phase p_1. Suppose the bar is uniformly in phase p_2 initially with one end fixed. We wish to subject the bar to an oscillating displacement and observe the phase transitions over time. The parameters that are measured are the strain, $w = u_x$, the velocity, $v = u_t$, and the order parameter, ϕ. This numerical experiment is similar to numerical experiments performed by Bubner [13]. Bubner explores solid-solid phase transition of CuZnAl single crystal with a triple-well potential. Bubner's model differs from ours in that it includes a higher order derivative of the displacement and does not include an order parameter.

In all our computations we choose a potential function with the center well below the outer wells. The function we use is the following polynomial

$$G(w) = -\frac{11}{144} + \frac{w^2}{2} + \frac{5w^4}{24} - \frac{29w^6}{18} + \frac{47w^8}{48} \tag{5.1}$$

which has local minima at $w = \pm 1$ and $w = 0$ which correspond to phases p_1, p_3 and p_2, respectively (see Figure 5.1). We assume initially that the bar is uniformly in phase p_1 and is at rest. This corresponds to the following initial conditions

$$w(x,0) = 0 \tag{5.2}$$
$$v(x,0) = 0 \quad x \in [0,1] \tag{5.3}$$
$$\phi(x,0) = 0. \tag{5.4}$$

One end of the bar is kept stationary while the velocity of the other end is required to oscillate. Our choice of boundary conditions is

$$w_x(0,t) = 0 \qquad w_x(1,t) = 0 \tag{5.5}$$
$$v(0,t) = 0 \qquad v(1,t) = a * sin(t) \quad t > 0 \tag{5.6}$$
$$\phi_x(0,t) = 0 \qquad \phi_x(1,t) = 0. \tag{5.7}$$

We first look at small oscillations about the trivial steady state. We choose γ such that the the free energy, ψ, defined by (2.32) is locally positive definite about the origin.

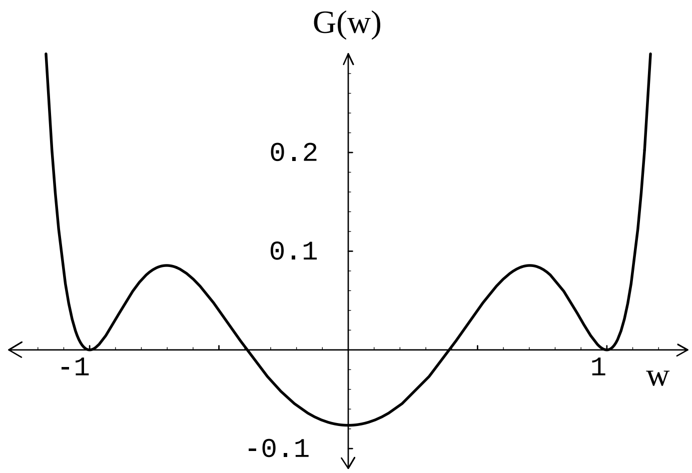

Figure 5.1: Triple-welled potential function $G(w)$.

We also choose a small amplitude for the loading function so as not to push w out of the middle well. Table 5.2 gives the parameters chosen for this first numerical experiment. As expected, w and ϕ show only slight variations over the time interval $[0, 2\pi]$ (see Figures 5.2 and 5.3). The variations are similar to linear wave motion.

Table 5.2: Parameters: no phase change

$\rho = 1$	$\beta = 1$	$\alpha = 1$	$\gamma = 0.9$
$\epsilon_1^2 = 0.0001$	$\epsilon_2^2 = 0.01$	$\epsilon_3^2 = 0.1$	$a = .1$

We next look at configurations for which the system generates phase transitions. We choose γ such that the free energy, ψ, defined by (2.32) is no longer positive definite about the origin. We also increase the amplitude of the load in order to push w out of the middle well. The value of ϵ_1^2 is increased for computational reasons. Table 5.3 gives the parameters chosen for this numerical experiment. The time interval is $[0, 6\pi]$. The strain, w, experiences two phase changes, from p_2 to both p_1 and p_3 (see Figure 5.4). The phase interface between p_1 and p_3 is sharp. The phase boundary after the initial phase change is smooth and mimics the forcing function as t increases. The order parameter, ϕ, also exhibits change from phase p_2 to p_1 and p_3 but does so in a smooth manner (see Figure 5.5).

We next consider the effect of nonhomogeneous initial conditions. We choose the initial conditions

$$\begin{aligned} w_0(x) &= 2\sin(20\pi x) \\ v_0(x) &= 0 \\ \phi_0(x) &= 2\sin(20\pi x). \end{aligned} \tag{5.8}$$

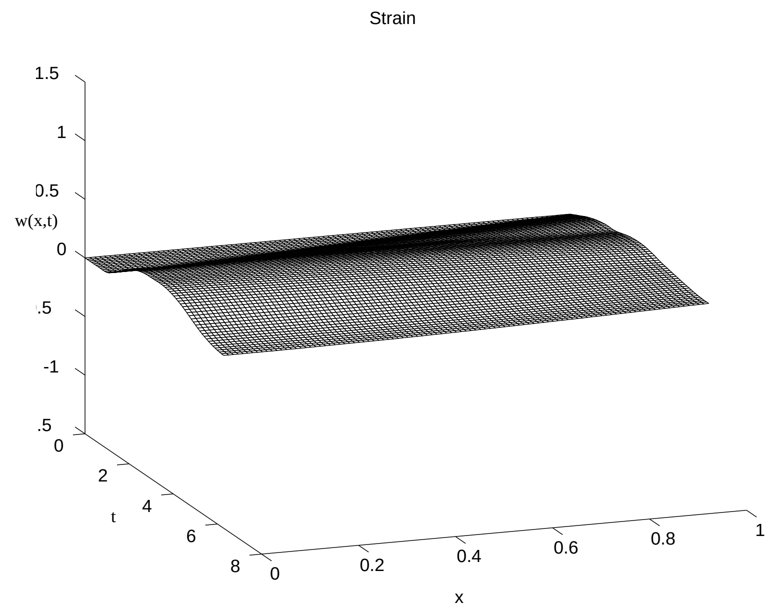

Figure 5.2: Strain: no phase transition.

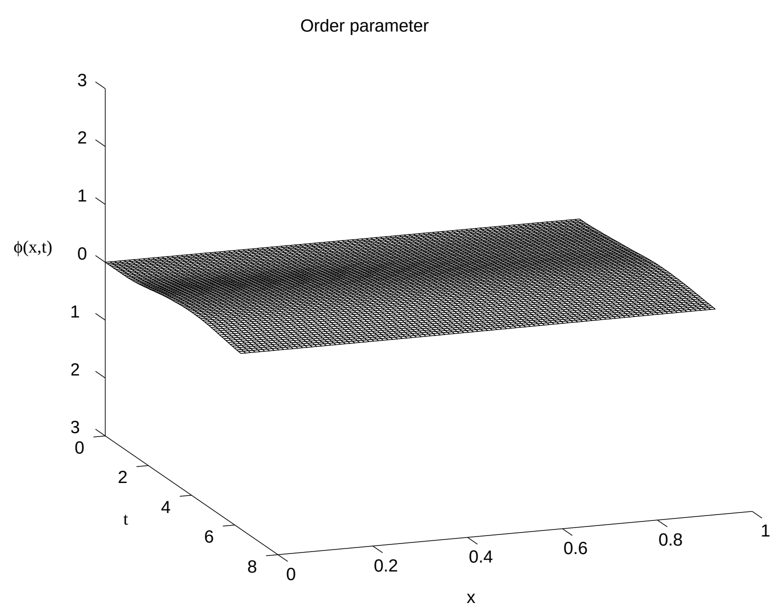

Figure 5.3: Order parameter: no phase transition.

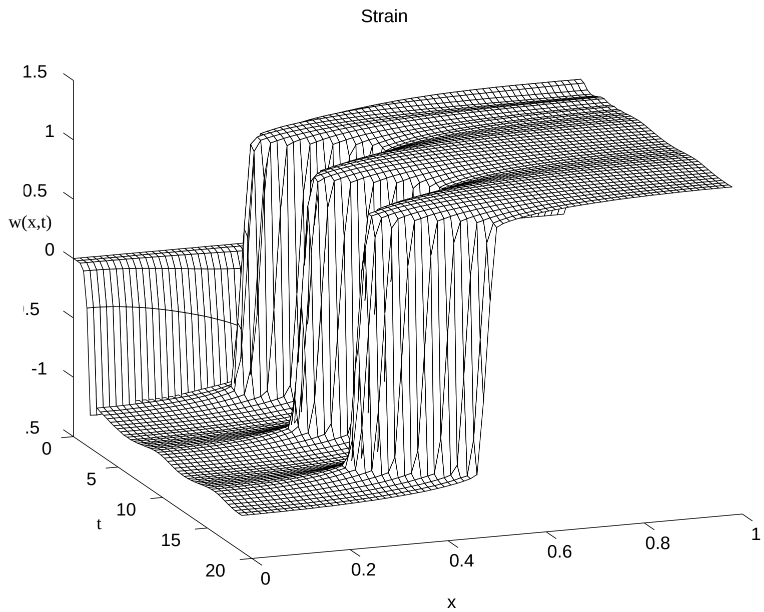

Figure 5.4: Strain: one phase boundary.

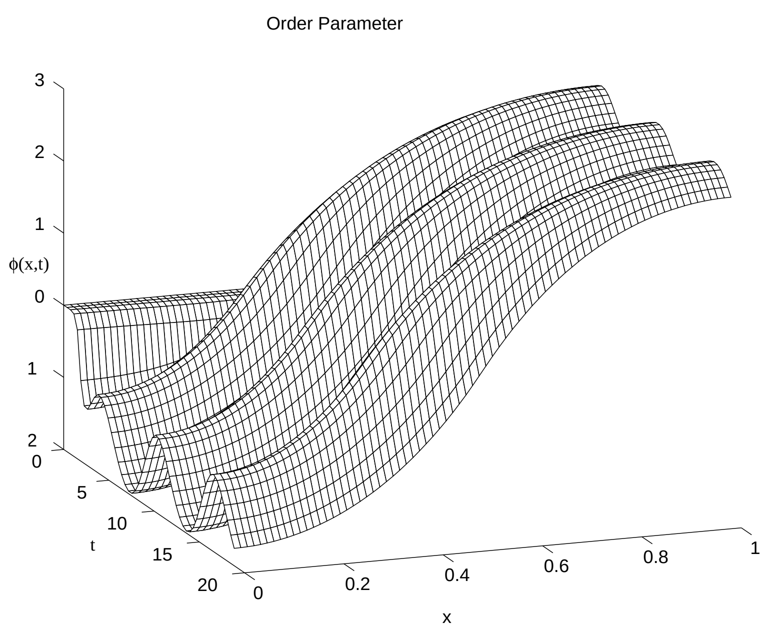

Figure 5.5: Order parameter: one phase boundary.

Table 5.3: Parameters: one phase transition.

$\rho = 1$	$\beta = 1$	$\alpha = 1$	$\gamma = 3$
$\epsilon_1^2 = 0.01$	$\epsilon_2^2 = 0.01$	$\epsilon_3^2 = 0.1$	$a = .25$

The initial conditions (5.8) are an attempt at forcing the material to exhibit microstucture. Table 5.4 gives the parameters chosen for this numerical experiment. The time interval is $[0, 1]$.

Table 5.4: Parameters: multiple phase transitions.

$\rho = 1$	$\beta = 1$	$\alpha = 1$	$\gamma = 3$
$\epsilon_1^2 = 0.01$	$\epsilon_2^2 = 0.01$	$\epsilon_3^2 = 0.05$	$a = .25$

This choice of initial conditions and parameters results in a solution symmetric about the midpoint that undergoes multiple phase transitions (see Figure 5.6). A contour map of the strain reveals an immediate transition from the microstucture to phase p_2 away from the endpoints. There is an immediate transition to a phase corresponding to an outer well at each endpoint with phase boundaries propagating toward the center (see Figure 5.7). The contour map also reveals two areas in the interior where two phase boundaries emanate from a single point. Each pair of phase boundaries propagate outward from their origin until they meet a second phase boundary. The solution has stabilized by time $t = 1$. Figure 5.8 shows the strain, w, at time $t = 0.44$ undergoing seven phase changes.

5.3 Comments

In his study of propagating phase boundaries in elastic bars of one dimension, James [71] considered the Riemann problem

$$w_t = v_x \tag{5.9}$$

$$v_t = \sigma'(w)w_x \quad (x,t) \in [-L, L] \times [0, T], \tag{5.10}$$

$$u_0(x) = \begin{cases} w_- & x \in [-L, 0] \\ w_+ & x \in (0, L]. \end{cases} \tag{5.11}$$

where w is the deformation, v is the velocity. The function $\sigma(\cdot)$ is the derivative of a non-convex stored energy (see Figure 5.9). On the interval $[\alpha^1, \beta^1]$, σ is unstable. On the region $[\alpha^*, \alpha^1) \cup (\beta^1, \beta^*], \sigma$ is metastable. For $u < \alpha^*$ or $u > \beta^*$, σ is stable.

James showed that there exist two kinds of solutions to the Riemann problem. The first is a one parameter family of solutions, each containing a single phase boundary. The

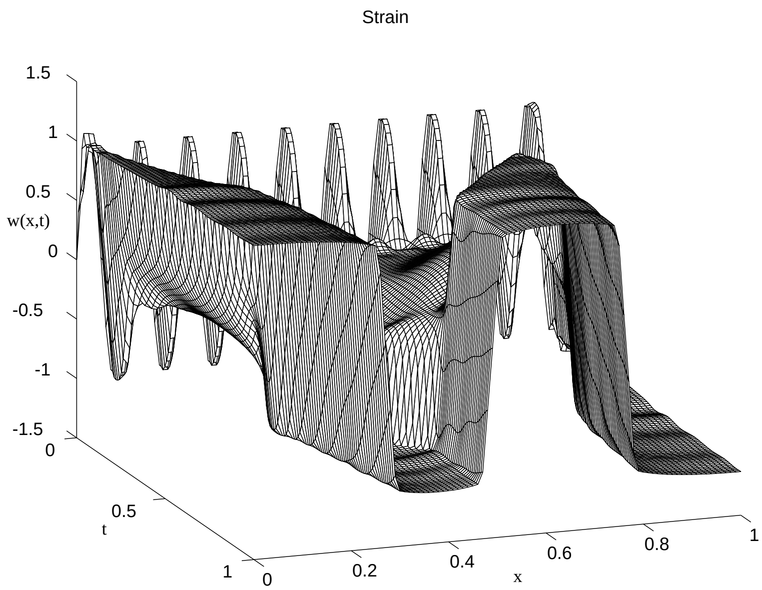

Figure 5.6: Strain: multiple phase boundaries.

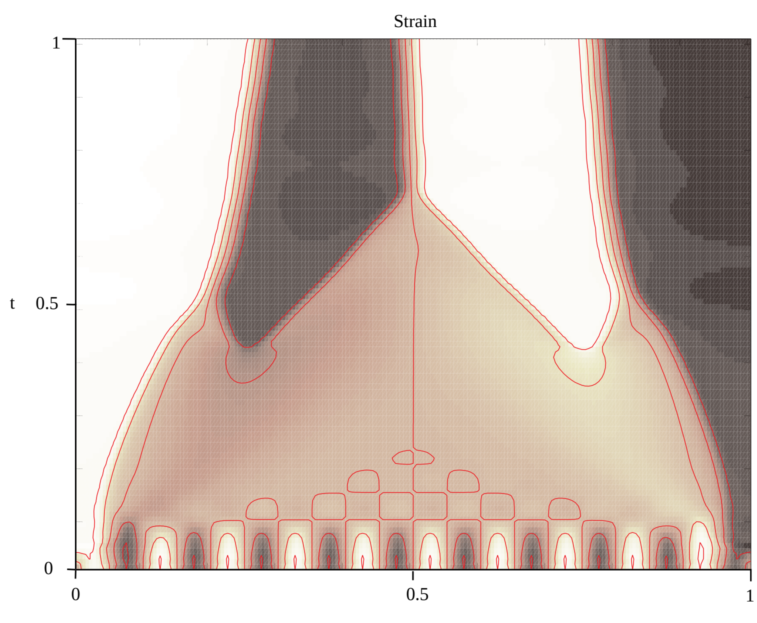

Figure 5.7: Strain: multiple phase boundaries.

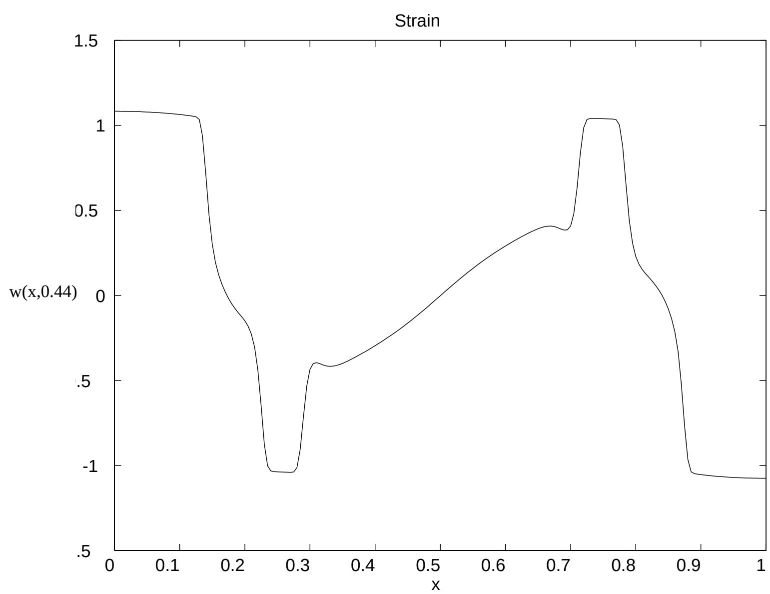

Figure 5.8: Strain at time $t = 0.44$: multiple phase boundaries.

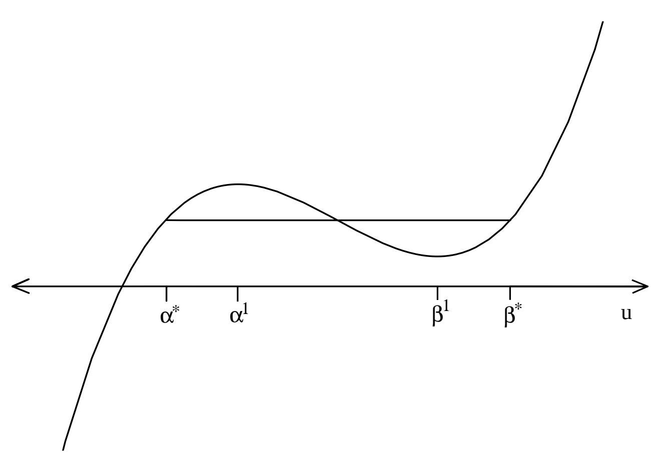

Figure 5.9: The function $\sigma'(u)$ and the Maxwell line.

second solution is a two parameter family of solutions containing two phase boundaries which emerge from constant initial data.

Equations (5.9) and (5.10) are very similar to (2.44) and (2.45),the first order system which describe the local balance law of momentum for the temperature independent model. Thus we should suspect that the Riemann problem for the system of equations (2.42) and (2.43) would also have families of solutions with one or two phase boundaries. However, since we solve a parabolic system, we expect a unique solution exhibiting similar characteristics of the solutions described by James. Indeed, we have seen such solutions in our computations e.g. Figure 5.7. We should point out that the solutions of the temperature dependent model with a phase boundary are solutions to a Riemann problem for some initial $t^* > 0$. The effect of including the viscosity terms, $\epsilon_1^2 w_{xx}$ and $\epsilon_2^2 v_{xx}$, in the first order system (2.44)-(2.46) is to isolate a particular member of the family of solutions. The value of ϵ_1^2 and ϵ_2^2 determine the family of solutions and the particular solution in that family.

Chapter 6

The Temperature Dependent Model

In this chapter we present an algorithm for the temperature dependent model (2.53)-(2.60) using a finite difference method in the space variable and Runge-Kutta method in the time variable and show the resulting numerical results.

6.1 A finite difference algorithm

In this section we present a description of an algorithm to solve the temperature dependent model (2.53)-(2.60). We use a finite difference method of $O(h^2)$ accuracy to discretize the space variable. We then apply a stage three Runge-Kutta method to the resulting differential equation in time.

To begin, we create a partition of $[a, b]$. Let N be a positive integer. We define the set of grid points $\Delta_{[a,b]}$ by

$$\Delta_{[a,b]} = \{a = x_0 < x_1 < \cdots < x_i < \cdots < x_{N-1} < x_N = b\}$$

where $x_i = a + ih, i = 0, 1, \cdots N$, and $h = \dfrac{(b-a)}{N}$. Let $u \in C^1((0, T); H^2(a, b))$. Let $t \geq 0$ be fixed. We discretize $u(x, t) = u(x)$ by using the $N + 1$ dimensional vector $\mathbf{u}$ where $u_i = u(x_i), 0 \leq i \leq N$. We use the following centered difference scheme to approximate u_x and u_{xx} at each interior node $x_i, 1 \leq i \leq N - 1$,

$$u_{i,x} = \frac{(u_{i+1} - u_{i-1})}{2h} \tag{6.1}$$

$$u_{i,xx} = \frac{(u_{i+1} - 2u_i + u_{i-1})}{h^2}. \tag{6.2}$$

It is a simple exercise in Taylor expansions to show that the above approximations are accurate up to $O(h^2)$.

Since we use Dirichlet boundary conditions for v and θ, we seek solutions only at the interior nodes, $x_i, 1 \leq i \leq N-1$. The Neumann boundary conditions for w and ϕ require solutions for each node. Therefore, let

$$\mathbf{u} = \begin{bmatrix} w_0 \\ \vdots \\ w_N \\ v_1 \\ \vdots \\ v_{N-1} \\ \phi_0 \\ \vdots \\ \phi_N \\ \theta_1 \\ \vdots \\ \theta_{N-1} \end{bmatrix}.$$

We wish to write our system of discretized equations as a system of first order differential equations in t, that is

$$\mathbf{u}_t(t) = \mathbf{F}(t, \mathbf{u}(t)). \tag{6.3}$$

We discretize the differential equations (2.53)-(2.56) for $1 \leq i \leq N-1$ using the centered difference approximations (6.1) and (6.2):

$$w_{i,t} = \frac{(v_{i+1} - v_{i-1})}{2h} + \epsilon_1^2 \frac{(w_{i+1} - 2w_i + w_{i-1})}{h^2} \tag{6.4}$$

$$\rho v_{i,t} = G_{ww}(w_i, \theta_i) \frac{(w_{i+1} - w_{i-1})}{2h} + G_{w\theta}(w_i, \theta_i) \frac{(\theta_{i+1} - \theta_{i-1})}{2h} \tag{6.5}$$

$$-\gamma \frac{(\phi_{i+1} - \phi_{i-1})}{2h} + \epsilon_2^2 \frac{(v_{i+1} - 2v_i + v_{i-1})}{h^2} \tag{6.6}$$

$$\beta \phi_{i,t} = \gamma w_i - \alpha \phi_i + \epsilon_3^2 \frac{(\phi_{i+1} - 2\phi_i + \phi_{i-1})}{h^2} \tag{6.7}$$

$$c\theta_{i,t} = \beta \phi_{i,t}^2 + \theta_i G_{\theta w}(w_i, \theta_i) \frac{(v_{i+1} - v_{i-1})}{2h} + k \frac{(\theta_{i+1} - 2\theta_i + \theta_{i-1})}{h^2}. \tag{6.8}$$

We must now discretize equations (2.53) and (2.55) about x_0 and x_N. We integrate equation (2.53) over the interval $[x_0, x_{\frac{1}{2}}]$ to get

$$\int_{x_0}^{x_{\frac{1}{2}}} w_t(x)dx = v(x)\big|_{x_0}^{x_{\frac{1}{2}}} + \epsilon_1^2 w_x(x)\big|_{x_0}^{x_{\frac{1}{2}}}.$$

We use the trapezoidal rule to approximate the integral on the left to get

$$\frac{h}{4}(w_t(x_{\frac{1}{2}}) + w_t(x_0)) = v(x_{\frac{1}{2}}) - v(x_0) + \epsilon_1^2 w_x(x_{\frac{1}{2}}) - w_x(x_0). \tag{6.9}$$

We may approximate the function values $v(x_{\frac{1}{2}})$ and $w_t(x_{\frac{1}{2}})$ by

$$v(x_{\frac{1}{2}}) = \frac{1}{2}(v(x_0) + v(x_1)) \tag{6.10}$$

$$w_t(x_{\frac{1}{2}}) = \frac{1}{2}(w_t(x_0) + w_t(x_1)). \tag{6.11}$$

Taylor expansions yield $O(h^2)$ accuracy for the above approximations. We use the centered difference equation (6.1) about $x_{\frac{1}{2}}$ and equations (6.10) and (6.11) in (6.9) to get

$$\frac{3h}{8} w_t(x_0) + \frac{3h}{w\ t}(x_1) = \frac{1}{2}(v(x_1) - v(x_0)) + \epsilon_1^2 \frac{(w(x_1) - w(x_0))}{h} - \epsilon_1^2 w_x(x_0)$$

or, in the vector notation,

$$\frac{3h}{8} w_{0,t} + \frac{h}{8} w_{1,t} = \frac{1}{2}(v_1 - v_0) + \epsilon_1^2 \frac{(w_1 - w_0)}{h} - \epsilon_1^2 w_{0,x}. \tag{6.12}$$

Using the same technique, we have

$$\frac{h}{8} w_{N-1,t} + \frac{3h}{8} w_{N,t} = \frac{1}{2}(v_N - v_{N-1}) + \epsilon_1^2 w_{N,x} - \epsilon_1^2 \frac{(w_N - w_{N-1})}{h} \tag{6.13}$$

$$\begin{aligned} \frac{3\beta h}{8} \phi_{0,t} + \frac{\beta h}{8} \phi_{1,t} &= \frac{\gamma h}{8}(w_1 + 3w_0) - \frac{\alpha h}{8}(\phi_1 + 3\phi_0) \\ &\quad + \epsilon_3^2 \frac{(\phi_1 - \phi_0)}{h} - \epsilon_3^2 \phi_{0,x} \end{aligned} \tag{6.14}$$

$$\begin{aligned} \frac{\beta h}{8} \phi_{N-1,t} + \frac{3\beta h}{8} \phi_{N,t} &= \frac{\gamma h}{8}(w_{N-1} + 3w_N) - \frac{\alpha h}{8}(\phi_{N-1} + 3\phi_N) \\ &\quad + \epsilon_3^2 \frac{(\phi_N - \phi_{-1})}{h} - \epsilon_3^2 \phi_{N,x} \end{aligned} \tag{6.15}$$

Since the trapezoidal rule for integrals is accurate up to $O(h^2)$, equations (6.12)-(6.15) are also accurate up to $O(h^2)$.

We define the function $G(t, \mathbf{u})$ using the right hand sides of equations (6.4)-(6.8) and (6.12)-(6.15), that is,

$$\begin{aligned} g_1(t, \mathbf{u}) &= \frac{1}{2}(v_1 - v_0) + \epsilon_1^2 \frac{(w_1 - w_0)}{h} - \epsilon_1^2 w_{0,x} \\ g_i(t, \mathbf{u}) &= \frac{(v_{i+1} - v_{i-1})}{2h} + \epsilon_1^2 \frac{(w_{i+1} - 2w_i + w_{i-1})}{h^2} \end{aligned}$$

$$
\begin{aligned}
g_N(t,\mathbf{u}) &= \frac{1}{2}(v_N - v_{N-1}) + \epsilon_1^2 w_{N,x} - \epsilon_1^2\frac{(w_N - w_{N-1})}{h} \\
g_{N+i}(t,\mathbf{u}) &= G_{ww}(w_i,\theta_i)\frac{(w_{i+1} - w_{i-1})}{2h} + G_{w\theta}(w_i,\theta_i)\frac{(\theta_{i+1} - \theta_{i-1})}{2h} \\
g_{2N}(t,\mathbf{u}) &= \frac{\gamma h}{8}(w_1 + 3w_0) - \frac{\alpha h}{8}(\phi_1 + 3\phi_0) + \epsilon_3^2\frac{(\phi_1 - \phi_0)}{h} - \epsilon_3^2\phi_{0,x} \\
g_{2N+i}(t,\mathbf{u}) &= \gamma w_i - \alpha\phi_i + \epsilon_3^2\frac{(\phi_{i+1} - 2\phi_i + \phi_{i-1})}{h^2} \\
g_{3N}(t,\mathbf{u}) &= \frac{\gamma h}{8}(w_{N-1} + 3w_N) - \frac{\alpha h}{8}(\phi_{N-1} + 3\phi_N) + \epsilon_3^2\frac{(\phi_N - \phi_{-1})}{h} - \epsilon_3^2\phi_{N,x} \\
g_{3N+i}(t,\mathbf{u}) &= \beta\phi_{i,t}^2 + \theta_i G_{\theta w}(w_i,\theta_i)\frac{(v_{i+1} - v_{i-1})}{2h} + k\frac{(\theta_{i+1} - 2\theta_i + \theta_{i-1})}{h^2}
\end{aligned}
$$

where $1 \le i \le N-1$. Thus we now have the Matrix equation

$$M\mathbf{u}_t = G(t,\mathbf{u})$$

where M is a tridiagonal constant coefficient matrix. We suppose M is invertible. Then we may define the function $F(t,\mathbf{u})$ by

$$F(t,\mathbf{u}) = M^{-1}G(t,\mathbf{u}).$$

We solve the differential equation using a stage three Runge-Kutta method. Let N be an integer. We define the time step τ by $\tau = \frac{T}{N}$. Set $\mathbf{u}^0 = \mathbf{u}(0)$. Then the solution is defined recursively by

$$\mathbf{u}^{m+1} = \mathbf{u}^m + \frac{1}{6}F_1 + \frac{2}{3}F_2 + \frac{1}{6}F_3$$

where

$$
\begin{aligned}
F_1 &= F(t^n, \mathbf{u}^n) \\
F_2 &= F(t^n + \frac{1}{2}F_1\tau, \mathbf{u}^m + \frac{1}{2}\tau F_1) \\
F_3 &= F(t^m + \tau, \mathbf{u}^m + \tau(-1F_1 + 2F_2))
\end{aligned}
$$

6.2 Numerical computations

In this section we present numerical results using the algorithm described in the previous section. We begin by presenting computational evidence that the finite difference method converges. We describe the numerical experiment and conclude with results.

We do not present error estimates for the finite difference algorithm developed in Section 6.1.1. However, we do test for convergence computationally. Choosing nonhomogeneous boundary and initial conditions which correspond to a known exact solution, we

Table 6.1: l^2 error for finite difference algorithm ($\times 10^{-3}$).

Number of steps	$N_t = 100$	$N_t = 400$	$N_t = 1600$
$N_x = 10$	2.6810	2.6800	2.6800
$N_x = 20$	NaN	0.92545	0.92543
$N_x = 40$	NaN	NaN	0.32343

solved the temperature independent system (2.53)-(2.55). We refine the number of space steps, N_x, and the number of time steps, N_t and look at the l^2 error, $e = \mathbf{u} - \mathbf{u}_h^N$, at time $t = t_N$ (see Table 6.1). The algorithm blows up if N_t is not large enough with respect to N_x. However, the algorithm provides solutions for which the error decreases at least linearly as N_x and N_t increase provided $N_t \geq N_x^2$. This type of error behavior is consistent with this type of Runge-Kutta finite difference method, e.g., see [46]. This yields a rather slow method. Implementation of a predictor/corrector method and or time step control most certainly would decrease computational time.

We now conduct a similar numerical experiment to that of Chapter 5 using the temperature dependent model. Consider a bar of unit length and uniform cross section of a material which has three natural solid phases, p_1, p_2 and p_3. Associated with this material is a symmetric triple-well potential, $G(w, \theta)$. The local minima, w_1 and w_3, of the outer wells correspond to phase, p_1 and p_3, respectively. The local minima, w_2, of the inner well corresponds to phase p_1. Suppose the bar is uniformly in phase p_2 initially with one end fixed. We wish to put the bar under an oscillating load and observe the phase transitions over time. The parameters which are measured are the strain, $w = u_x$, the stress, $v = u_t$, the order parameter, ϕ, and the temperature, θ.

In our computation we choose the following potential function

$$G(w) = \frac{25 - 36\theta}{144} + \frac{\theta w^2}{2} + \frac{5w^4}{24} - \frac{(20 + 9\theta)w^6}{18} + \frac{(35 + 12\theta)w^8}{48} \tag{6.16}$$

which has local minima at $w = \pm 1$ and $w = 0$ which correspond to phases p_1, p_3 and p_2, respectively (see Figure 5.1). The height of the middle well is determined by θ (see Figure 6.1). We assume initially that the bar is uniformly in phase p_1 and is at rest. We also assume that the initial temperature is a linear function in x. This corresponds to the following initial conditions

$$w(x, 0) = 0 \tag{6.17}$$
$$v(x, 0) = 0 \tag{6.18}$$
$$\phi(x, 0) = 0 \tag{6.19}$$
$$\theta(x, 0) = x + 1 \tag{6.20}$$

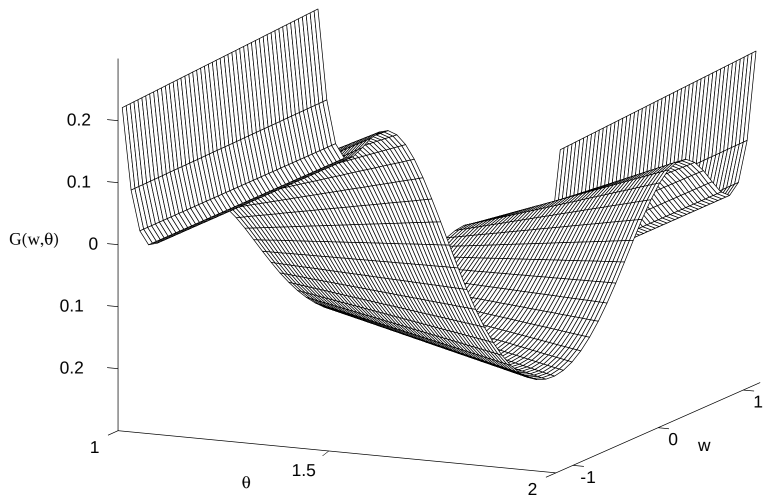

Figure 6.1: Triple-welled potential function $G(w, \theta)$.

for $x \in [0, 1]$. One end of the bar is kept stationary while an oscillating load is applied to the free end over time. We assume there is no change in the strain, the phase nor the temperature at the ends of the bar throughout time. Our choice of boundary conditions is

$$w_x(0,t) = 0 \qquad w_x(1,t) = 0 \tag{6.21}$$
$$v(0,t) = 0 \qquad v(1,t) = a * sin(t) \tag{6.22}$$
$$\phi_x(0,t) = 0 \qquad \phi_x(1,t) = 0 \tag{6.23}$$
$$\theta(0,t) = 1 \qquad \theta(1,t) = 2 \tag{6.24}$$

for $t > 0$. The initial condition 6.20) and the boundary conditions (6.24) for θ imply that the shape of G will vary as x increases, that is, as $x \to 0, \theta$ also increases and, hence, the depth of the center well of G increases (see Figure 6.2).

We look at at small oscillations about the trivial steady state. We choose γ such that the the free energy, ψ, defined by (2.32) is locally positive definite about the origin. We also choose a small amplitude for the loading function so as not to push w out of the middle well at the free end of the bar. Table 6.2 gives the parameters chosen for this first numerical experiment. As expected, w and ϕ show only slight variations over the time interval $[0, 2\pi]$ near the free end. The change in both w and ϕ increase as x approaches 0 and the middle well of G rises (see Figures 6.3 and 6.4). The temperature appears to have not changed at all (see Figure 6.5).

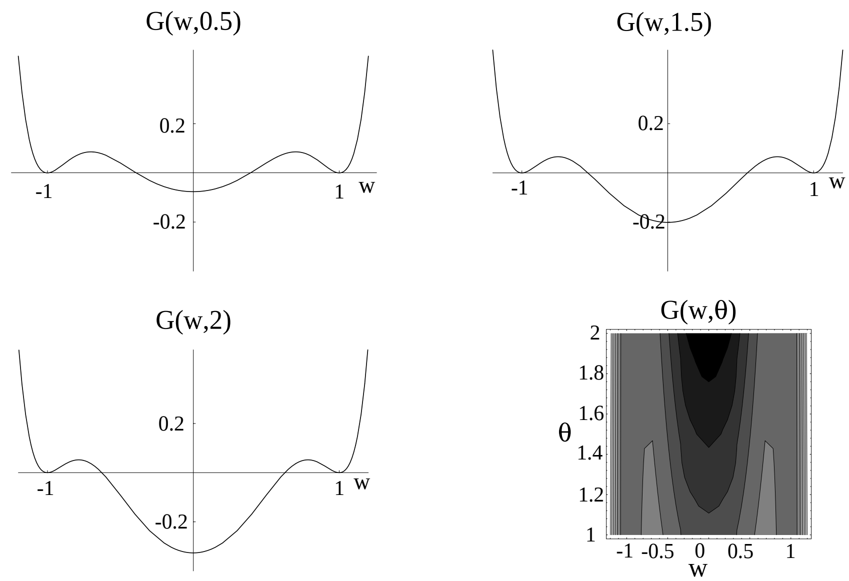

Figure 6.2: Triple-welled potential function $G(w, \theta)$.

Table 6.2: Parameters: temperature dependent model.

$\rho = 1$	$\beta = 1$	$\alpha = 1$	$\gamma = 0.9$	$c = 0.4$
$\epsilon_1^2 = 0.01$	$\epsilon_2^2 = 0.01$	$\epsilon_3^2 = 0.1$	$k = 2$	$a = .1$

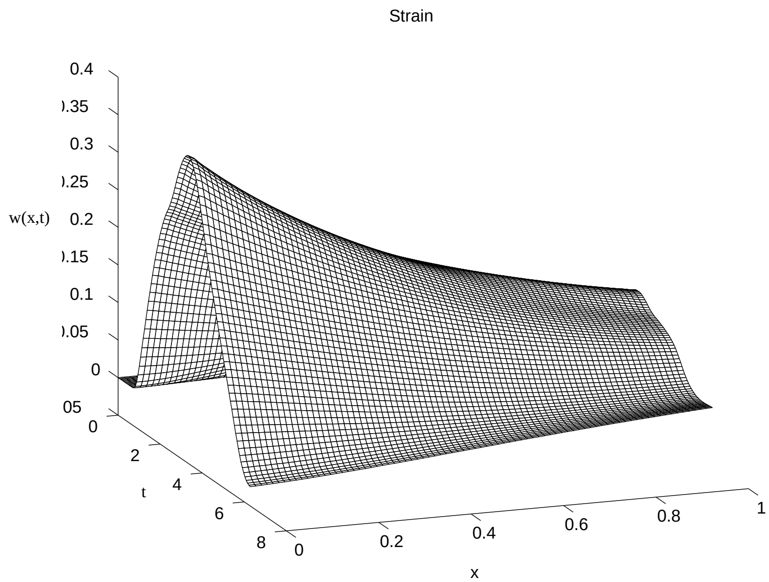

Figure 6.3: Strain: temperature dependent model.

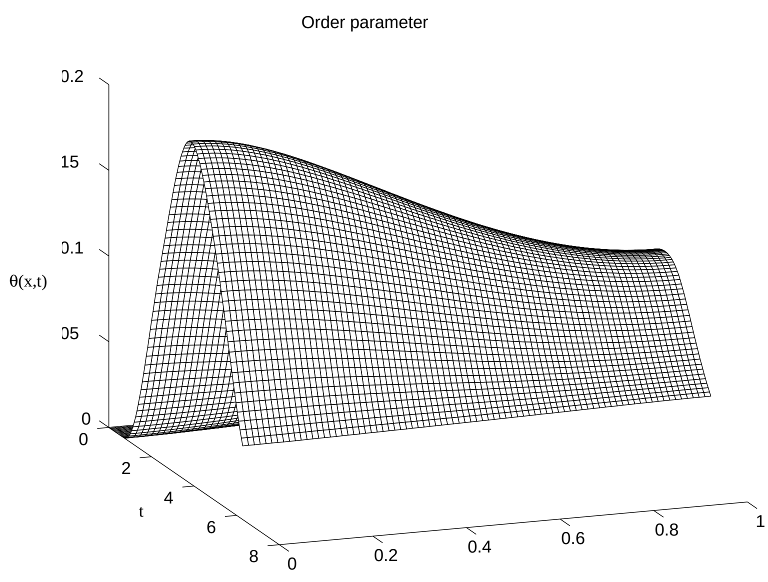

Figure 6.4: Order parameter: temperature dependent model.

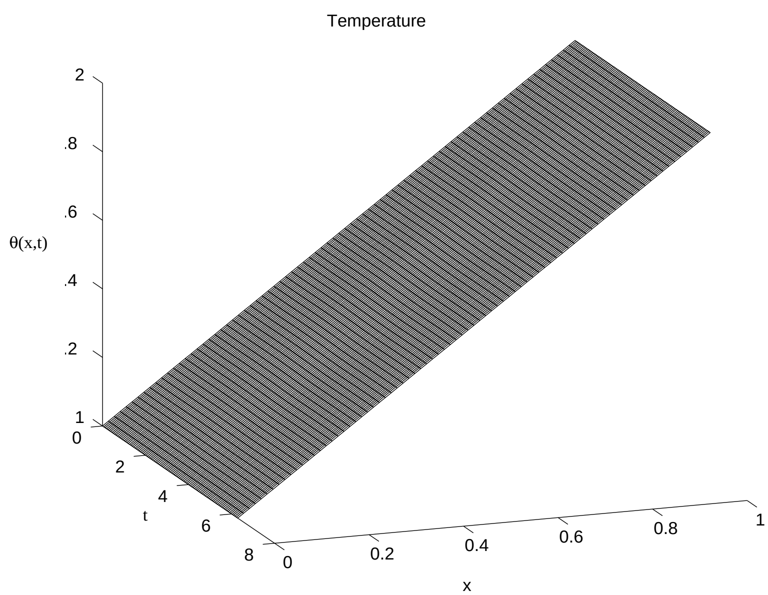

Figure 6.5: Temperature: temperature dependent model.

Chapter 7

Future inquiries

In this chapter we discuss open problems related to the order parameter model of phase transition discussed in this thesis and work yet to be done. There is much analysis yet to be done for both the existence theory and the numerical theory. In addition, our numerical investigation of the physics of solid-solid phase transition has only just begun. There are variations of the model that may be investigated. These variations would result from alternative choices in the derivation of the model, either in the choice of global balance laws or in the choice of the constitutive functions. The following list expands on the above discussion.

- We presented existence theory and numerical analysis of the finite element method for the simplest of problem, that of homogeneous Dirichlet boundary conditions, yet we computed solution using non-constant Dirichlet and Neumann boundary conditions. The question of existence and uniqueness of the latter problem has yet to be considered.

- We have not addressed the question of existence of a solution for the temperature independent system. We cannot apply the techniques used in Chapter 3 due to the nonlinear term ϕ_t^2 in equation (2.56). Thus we must use an alternative approach for proving that a solution exists.

- We did not derive error estimates for the fully discretized finite element algorithm presented in Chapter 4. It should be fairly straightforward to show that the error is of order $h + \tau$ assuming the solution $\mathbf{u}$ is smooth enough. It may be possible to obtain higher higher order error estimates.

- We have investigated the mathematics of the model, albeit the simplest of cases, but we have only just touched upon the numerical study of the physics. For example, our numerical investigation of the temperature independent model only included one choice for G where the center well is below the outer two wells. We have yet to explore other choices for G.

- In the case of the temperature dependent model, we have done virtually nothing other than establish that our numerical algorithm will converge and that the resulting numerical solutions seem reasonable. The values we choose for the parameters are arbitrarily. We do not know if they represent the actual physics of materials undergoing solid-solid phase transitions.

- A possible variation in the derivation of the model is to include a momentum term in the global balance law of microlocal forces (2.2) of the form

$$\frac{\partial}{\partial t}\int_a^b c(x)\phi_t(x,t)dx \tag{7.1}$$

where $c(\cdot)$ is a density function. Why Gurtin and Fried [61] [63] chose not to include this momentum term is not clear. One possible explanation is that by ignoring the momentum term, the resulting phase transition model reduces to the phase field model upon choosing specific parameters. A consequence of adding the momentum term (7.1) to the global balance law of microlocal forces (2.2) is that the resulting partial differential equations would include a second order derivative of ϕ with respect to t. This should allow us to prove the existence and uniqueness of a solution to the temperature dependent model applying the techniques used in Section 3.3. In addition, a finite element algorithm similar to that derived in Section 4.3 would be feasible as the nonlinear term involving ϕ_t would include lower order derivatives.

- Another variation in the derivation of the model is the constitutive choice of the free energy function ψ. Recent study by Salje [90] of phase transition of crystal lattices suggests that the nonlinearity term in the free energy, ψ, be dependent on ϕ, ϕ_x and u_x. That being so, the study of the temperature independent model in this thesis would be one of many specific models to be studied.

Bibliography

[1] Stuart S. Antman. *Nonlinear Problems of Elasticity*, volume 107 of *Applied Mathematical Sciences*. Springer Verlag, New York, 1995.

[2] J.M. Ball and R.D. James. Fine phase mixtures as minimizers of energy. *Archives of Rational Mechanics and Analysis*, 100:13–52, 1987.

[3] P.W. Bates and P. Fife. The dynamics of nucleation for the Cahn-Hilliard equation. *SIAM Journal of Applied Mathematics*, 54(4):990–1008, August 1993.

[4] P.W. Bates and P.C. Fife. Spectral comparison principles for the Cahn-Hilliard and phase field equations and time scales for coarsening. *Physica D*, 43:335–348, 1990.

[5] W.J. Boettinger, R. Kobayashi, G.B. McFadden, B.T. Murray, and A.A. Wheeler. *A Phase Field, Diffuse Interface Solidification Models for Pure Metals and Binary Alloys.* The Minerals,Metals and Materials Society, 1993.

[6] W.J. Boettinger, G.B. Mcfadden, and A.A. Wheeler. Phase-field model for isothermal phase transition in binary alloys. *Physical Review A*, 45(10):7424–7439, May 1992.

[7] W.J. Boettinger, G.B. Mcfadden, and A.A. Wheeler. Phase field model of solute trapping during solidification. *Physical Review E*, 47(3):1893–1909, March 1993.

[8] W.J. Boettinger and A.A. Wheeler. *Toward a Phase Field Model for Phase Transitions in a Binary Alloy.*, pages 127–136. Springer-Verlag, N.Y., 1992.

[9] D. Brandon, T. Lin, and R.C. Rogers. Phase transitions and hysteresis in nonlocal and order parameter models. *Meccanica*, 30:541-565, 1995.

[10] D. Brandon and R.C. Rogers. Order parameter models of elastic bars and precursor oscillations. Technical Report 1370, IMA, November 1995.

[11] R.J. Braun, S.R. Coriell, G.B. McFadden, B.T. Murray, R.F. Sekerka, S.L. Wang, and A.A. Wheeler. Thermodynamically consistent phase field models for solidification. *Physica D*, 69:189–200, 1993.

[12] R.J. Braun, S.R. Coriell, G.B. Mcfadden, R.F. Sekerka, and A.A. Wheeler. Phase-field models for anisotropic interfaces. *Physical Review E*, 48(3):2016–2024, September 1993.

[13] Nikolaus Bubner. Landau-Ginzburg model for a deformation-driven experiment on shape memory alloys. Weierstass-Institut fur Angewandte Analysis und Stochastik. Berlin., September 1995.

[14] G. Caginalp. An analysis of a phase field model of a free boundary. *Archives of Rational Mechanics and Analysis*, 92:205–245, 1986.

[15] G. Caginalp. Conserved-phase field system: Implications for kinetic supercooling. *Physical Review B*, 38(1):789–791, July 1988.

[16] G. Caginalp. Stefan and Hele-Shaw type models as asymptotic limits of the phase-field equations. *Physical Review A*, 38(11):5887–5896, June 1989.

[17] G. Caginalp. The dynamics of a conserved phase field system: Stefan-like Hele-Shaw and Cahn-Hilliard models as asymptotic limits. *IMA Journal of Applied Mathematics*, 44:77–94, 1990.

[18] G. Caginalp. Phase field models and sharp interface limits: Some differences in subtle situations. *Rocky Mountain Journal of Mathematics*, 21(2):603–616, 1991.

[19] G. Caginalp. *The Issues of Anisotropy and Traveling Wave Velocity Selection in the Phase Field Model.*, pages 92–95. Longman Scientific and Technical, Harlow,UK, 1993.

[20] G. Caginalp and Xinfu Chen. *Phase Field Equations in the Singular Limit of Sharp Interface Problems.*, pages 1–28. Springer-Verlag, N.Y., 1992.

[21] G. Caginalp and P. Fife. Higher-order phase field models and detailed anisotropy. *Physical Review B*, 34(7):4940–4943, October 1986.

[22] G. Caginalp and P. Fife. Elliptic problems involving phase boundary satisfying a curvature condition. *Journal of Applied Mathematics*, 87:195–217, 1987.

[23] G. Caginalp and P. Fife. Dynamics of layered interfaces arising from phase boundaries. *SIAM Journal of Applied Mathematics*, 48(3):506–518, June 1988.

[24] G. Caginalp and S. Hastings. Properties of some ordinary differential equations related to free boundary problems. *Proceedings of the Royal Society of Edinburgh*, 104A:217–234, 1986.

[25] G. Caginalp and J. Jones. *A Phase Field Model: Derivation and New Interface Relation.*, pages 29–50. Springer-Verlag, N.Y., 1992.

[26] G. Caginalp and J.T. Lin. A numerical analysis of an anisotropic phase field model. *IMA Journal of Applied Mathematics*, 39:51–66, 1987.

[27] G. Caginalp and Y. Nishiura. The existence of traveling waves for phase field equations and convergence to sharp interface models in the singular limit. *Quarterly of Applied Mathematics*, 49(1):147–162, March 1991.

[28] G. Caginalp and Fife P. Phase-field models for interfacial boundaries. *Physical Review B*, 33(11):7792–7794, June 1986.

[29] G. Caginalp and E.A. Socolovsky. Computation of sharp phase boundaries by spreading the planar and spherically symmetric cases. *Journal of Computational Physics*, 95:85–100, 1991.

[30] G. Caginalp and E.A. Socolovsky. Efficient computation of interface and instabilities by smoothing via phase field methods. Advances in Mathematics, Computations and Reactor Physics, 1991.

[31] G. Caginalp and E.A. Socolovsky. Phase field computations of single-needle crystals, crystal growth and motion by mean curvature. *SIAM Journal of Scientific and Statistical Computing*, 1994 to appear.

[32] G. Caginalp and W. Xie. Phase field and sharp interface alloy models. *Physical Review E*, 48(3):1897–1909, September 1993.

[33] John W. Cahn. On spinodal decomposition in cubic crystals. *Acta Metallurgica*, 10:179–183, 1962.

[34] John W. Cahn. Phase separation by spinodal decomposition in isotropic systems. *J. of Chemical Physics*, 42:93–99, 1965.

[35] John W. Cahn. Spinodal decomposition. *Trans. Metallurg. Soc. of AIME*, 242:166–180, 1968.

[36] J.W. Cahn. On spinodal decomposition. *Acta Metallurgica*, 9:795–801, September 1961.

[37] J.W. Cahn and J.E. Hilliard. Free energy of a nonuniform system. I. interface free energy. *Journal of Chemical Physics*, 28(2):258–267, February 1958.

[38] Jack Carr, Mortin E. Gurtin, and Marshall Slemrod. Structured phase transitions on a finite interval. *Archives of Rational Mechanics and Analysis*, 86(4):317–351, 1984.

[39] Zhiming Chen. Optimal boundary controls for a phase field models. Technical Report 432, Institut fur Angewandte Mathematik und Statistik, Technische Universitat Munchen, Munchen, Germany, 1993.

[40] Zhiming Chen and K.H. Hoffmann. An error estimate of a finite element scheme for a phase field model. Technical report, Institut fur Angewandte Mathematik und Statistik, Technische Universitat Munchen, Postfach 20 10 32 D–80010 Munchen, Germany, 1991.

[41] Zhiming Chen and K.H. Hoffmann. *Numerical solutions of the optimal control problem governed by a phase field model.*, volume 100 of *International Series of Numerical Mathematics*. Birkhauser Verlag, Germany, 1991.

[42] P.G. Ciarlet. *The Finite Element Method for Elliptic Problems.* North-Holland, Amsterdam, 1978.

[43] Earl A. Coddington and Norman Levinson. *Theory of Ordinary Differential Equations.* McGraw-Hill, New York, 1955.

[44] Bernard D. Coleman and Walter Noll. The thermodynamics of elastic materials with heat conduction and viscosity. *Archives of Rational Mechanics and Analysis*, 13:167–178, 1963.

[45] Joseph B. Collins and Herbert Levine. Diffuse interface model of diffusion-limited crystal growth. *Physical Review B*, 31(9):6119–6122, 1985.

[46] John R. Dormand. *Numerical Methods for Differential Equations.* CRC Press, New York, 1996.

[47] C.M. Elliott. *The Cahn-Hilliard model for the kinetics of phase separation.*, pages 35–73. in: Mathematical Models for Phase Change Problems, J.F. Rodrigues, ed. Int. Ser. of Numerical Mathematics, Vol. 88, Birkhauer Verlag, Basel. 1989.

[48] C.M. Elliott and D.A. French. Numerical studies of the Cahn-Hilliard equation for phase separation. *IMA Journal of Applied Mathematics*, 38:97–128, 1987.

[49] C.M. Elliott and A.R. Gardiner. *One Dimensional Phase Field Computations.*, pages 56–74. Layman Scientific and Technical, 1993.

[50] C.M. Elliott and S. Zheng. On the Cahn-Hilliard equation. *Archives of Rational Mechanics and Analysis*, 96:339–357, 1986.

[51] P. Fife. Pattern dynamics for parabolic pde's. In *Introduction to Dynamical Systems.* IMA, Springer, Sep. 1989. to appear.

[52] P. Fife. Models for phase separation and their mathematics. 1991.

[53] P. Fife and G.S. Gill. The phase field description of mushy zones. *Physica D*, 35:267–275, 1989.

[54] P. Fife and G.S. Gill. Phase transition mechanisms for the phase field model under internal heating. *Physical Review A*, 43(2):843–851, January 1991.

[55] P. Fife and O. Penrose. Thermodynamically consistent models of phase field type for the kinetics of phase transitions. *Physica D*, 43:44–62, 1990.

[56] P. Fife and O. Penrose. On the relation between the standard phase field model and a "thermodynamically consistent" phase field model. *Physica D*, 69:107–113, 1993.

[57] George J. Fix. *Phase Field Methods for Free Boundary Problems.*, pages 580–589. Pitman, Boston, 2 edition, 1983.

[58] G.J. Fix and J.T. Lin. Numerical simulations of nonlinear phase transitions: 1. the isotropic case. *Nonlinear Analysis, Theory, Methods & Applications*, 12(8):811–823, 1988.

[59] I. Fonseca and L. Tartar. The gradient theory of phase transitions for systems with two potential wells. *Proceedings of the Royal Society of Edinburgh Year=1986*, 111A:89–102, 1989.

[60] E. Fried. Continuum theory for coherent phase transitions incorporating an order parameter. 1994.

[61] E. Fried and M.E. Gurtin. Continuum theory of thermally induced phase transitions based on an order parameter. *Physica D*, 68:326–343, 1993.

[62] E. Fried and M.E. Gurtin. Continuum phase transitions with an order parameter; accretion and heat conduction. 1994.

[63] E. Fried and M.E. Gurtin. Dynamic solid-solid transition with phase characterized by an order parameter. *Physica D*, 72:287–308, 1994.

[64] J.W. Gibbs. On the equilibrium of heterogeneous substances. Transactions of the Connecticut Academy,III. pp.108-248, Oct. 1875-May, 1876, and pp.343-524, May, 1877-July, 1878. Reprinted in J.W.Gibbs,. Reprinted in J.W. Gibbs, *Collected Works*, Vol. 1, pp. 56-353, Longman, New York, 1928. (Reprinted by Dover, 1961).

[65] M.E. Gurtin. On phase transitions with bulk, interfacial, and boundary energy. *Archives of Rational Mechanics and Analysis*, 96:243–264, 1986.

[66] B.I. Halperin and P.C. Hohenberg. Theory of dynamic critical phenomena. *Review of Modern Physics*, 49(3):435–475, July 1977.

[67] B.I. Halperin, P.C. Hohenberg, and S.K. Ma. Renormalization-group methods for critical dynamics: 1 recursion relations and effects of energy conservation. *Physical Review B*, 10(1):139–153, 1974.

[68] Dan Henry. *Geometric Theory of Semilinear Parabolic Equations*, volume 840 of *Lecture Notes in Mathematics*. Springer Verlag, New York, 1981.

[69] Werner Horn. A numerical scheme for the one-dimensional, Penrose-Fife model for phase transitions. Technical Report 381, Anwendungsbezogere Optimierung und Steuerung, Universitat -GH Essen, Essen, Germany, 1992.

[70] Werner Horn, Philippe Laurencot, and Jurgen Sprekels. Global solutions to a Penrose-Fife phase-field model under flux boundary conditions for the inverse temperature. March 1994.

[71] Richard D. James. The propagation of phase boundaries in elastic bars. *Archives of Rational Mechanics and Analysis*, 73(2):125–158, 1980.

[72] N. Kenmochi and M. Niezgodka. Evolution systems of nonlinear variational inequalities arising from phase change problems. *Nonlinear Analysis TMA* to appear.

[73] N. Kenmochi and M. Niezgodka. Systems of nonlinear parabolic equations for phase change problems. *Adv. Math. Sci. Appl.* to appear.

[74] N. Kenmochi and M. Niezgodka. *System of variational inequality arising in nonlinear diffusion with phase change.*, volume 106 of *International Series of Numerical Mathematics*. Birkhauser Verlag, Berlin, 1992.

[75] Ryo Kobayashi. *Simulations of Three Dimensional Dendrites.*, pages 121–128. World Scientific, London, 1992.

[76] Ryo Kobayashi. Modeling and numerical simulations of dendritic crystal growth. *Physica D*, 63:410–423, 1993.

[77] Tao Lin and Robert C. Rogers. Computations of phase transitions using non-local regularization. 1993.

[78] Tao Lin and Robert C. Rogers. On an order parameter model for a binary liquid. 1994.

[79] Gérard Maugin and Wolfgang Muschik. Thermodynamics with internal variables: Part I. General concepts. *J. Non-Equilib. Thermodyn*, 19:217–249, 1994.

[80] Gérard Maugin and Wolfgang Muschik. Thermodynamics with internal variables: Part II. Applications. *J. Non-Equilib. Thermodyn*, 19:250–289, 1994.

[81] J.C. Maxwell. Capillary action. *Encyclopedia Britannica, 9th ed.*, 1876. (Reprinted in *The Scientific Papers of James Clerk Maxwell*, W.D. Niven, ed., Vol. 2, pp. 541-591. Dover, New York, 1954.).

[82] L. Modica. The gradient theory of phase transitions and the minimal interface criterion. *Archives of Rational Mechanics and Analysis*, 98(2):123–142, 1987.

[83] B.T. Murray, R.J. Scheafer, and A.A. Wheeler. Computation of dendrites using a phase field model. *Physica D*, 66:243–262, 1993.

[84] A. Pazy. *Semigroups of Linear Operators and Applications to Partial Differential Equations.*, volume 44 of *Applied Mathematical Sciences*. Springer Verlag, New York, 1983.

[85] Robert L. Pego. Front migration in the nonlinear Cahn-Hilliard equation. *Proc. Roy. Soc. of London A*, 422:261–278, 1989.

[86] O. Penrose. *Statistical mechanics and the kinetics of phase separation.*, pages 373–394. in: Material Instabilities in Continuum Mechanics and Related Mathematical Problems, J.M. Ball, ed. Claendon Press. 1988.

[87] M. Renardy and R.C. Rogers. *An Introduction to Partial Differential Equations*, volume 13 of *Texts in Applied Mathematics*. Springer Verlag, New York, 1992.

[88] J.S. Rowlinson. Translation of J.D. van der Waals' the thermodynamic theory of capillarity under the hypothesis of a continuous variation of density. *J. of Statistical Physics*, 20:197–244, 1979.

[89] L.I. Rubenstien. *The Stefan problem.* Translations of Mathematical Monographs, Vol. 27, Providence, RI, 1971.

[90] E.K.H. Salje. *Phase Transitions in Ferroelstic and Co-Elastic Crystals*. Cambridge University Press, 1993.

[91] T.W. Shield. Orientation dependence of the psuedoelastic behavior of single crystals of Cu-Al-Ni in tension. Submitted to the *J. of the Mechanical and Physical*, September 1994.

[92] J. Sprekels and Songmu Zheng. Global smooth solutions to a thermodynamically consistent model of phase field type in higher space dimensions. *Journal of Mathematical Analysis and Applications*, 176:200–223, 1993.

[93] Vidar Thomee. *Galerkin Finite Element Methods for Parabolic Problems*, volume 1054 of *Lecture Notes in Mathematics*. Springer Verlag, New York, 1984.

[94] J.D. Van der Waals. On the thermodynamic theory of capillarity under the hypothesis of continuous variation of density. (in dutch). *Verhandel. Konink. Akad. Weten. Amsterdam*, 1, (Sect. 1) 1893. (See [88] for an English translation).

[95] Mary Fanett Wheeler. A priori l_2 error estimates for galerkin approximations to parabolic partial differential equations. *SIAM Journal of Numerical Analysis*, 10(4):723–759, September 1973.

[96] Eberhard Zeidler. *Nonlinear Functional analysis and its Applications II/A: Linear Monotone Operators*. Springer Verlag, New York, 1990.

[97] Songmu Zheng. Asymptotic behavior of the solution to the Cahn-Hilliard equation. *Appl. Anal.*, 23:165–184, 1986.

[98] Songmu Zheng. Global existence for a thermodynamically consistent model of phase field type. *J. of Diff. Integral Equations*, 5:241–253, 1992.

VITA

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